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COMPUTER MODELLING, SIMULATION AND CONTROL OF A KAMYR CONTINUOUS DIGESTER

by

© KHAWAJA MOAZZAM RAHMAN

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES AND RESEARCH

IN PARTIAL FULFILMENT OF THE REQUIREMENTS FOR THE DEGREE

OF MASTER OF SCIENCE

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SPRING 1979

THE UNIVERSITY OF ALBERTA

FACULTY OF GRADUATE STUDIES AND RESEARCH

The undersigned certify that they have read, and recommend to the Faculty of Graduate Studies and Research, for acceptance, a thesis entitled COMPUTER MODELLING SIMULATION AND CONTROL OF A KAMYR CONTINUOUS DIGESTER submitted by KHAWAJA MOAZZAM RAHMAN in partial fulfilment of the requirements for the degree of Master of Science in Chemical Engineering.

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Date.....December 1, 1978..

ABSTRACT

This thesis is the first study in a bleached pulp and paper mill modelling and control project in the Department of Chemical Engineering, University of Alberta. A nonlinear lumped parameter model for a Kamyr continuous kraft pulping digester was developed. This model includes thirteen state variables which include: the wood flow rate, wood component concentrations and entrapped and free liquor concentrations. The digester is split up into a number of sections each of which are an ideal stirred tank. These sections are further divided into three subsections that include diffusion of cooking chemicals and reaction products from the chip. The subsections are for wood, entrapped liquor in the wood and the free liquor flowing in the chip void volume. The nonlinear set of ordinary differential equations are solved for each section in the digester, including the digester washing sections.

The complete digester modelling package consists of a dynamic and steady state representation of a continuous digester and one of a batch digester. The continuous digester model testing was done in parts. Individual modules of the program were tested first, followed by

testing of the overall program for which the final results were known. The validity of the kinetic cooking model was compared using the batch digester model that was developed for the purpose. The dynamic program was checked by running the digester from starting with a constant initial profile and continuing to the final steady state and comparing this with the results obtained from the steady state model.

Dynamic open loop simulation runs for the Kamyr digester were conducted with the ultimate aim of evaluating various industrial control practices. The three main operating control variables are cooking temperature, cook zone residence time and cooking chemical concentration. These variables were varied to evaluate different operating tradeoffs and the effect on scalar measures that are used for pulp quality characterization, such as H-Factor, residual lignin content, Kappa number. The H-Factor, for example, that incorporates cooking time and temperature was found to be inadequate when large alkali concentration changes were involved and the residual lignin content (Kappa number) was similar although significantly different operating conditions were used. This led to the hypothesis that "profile control" was better and more reliable compared to control using a scalar quantity. The implementation of this concept should be practical considering the current

availability of computer hardware and technology.

Open loop feedforward type of control was studied for a chip species change and a production rate change. Finally typical digester closed loop control schemes are reviewed and presented.

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CHAPTER ONE

INTRODUCTION

A pulp and paper mill modelling and control study was undertaken to provide a basis for further work in the field at the Department of Chemical Engineering. Pulp and paper production is an important segment of Canadian industry and it was felt that the area was a late starter in computer control, especially when compared with the petroleum related industries. It was also observed that this trend was bound to shift in the future as faster minicomputers and better sensors became available. It was also obvious that in the meantime a lot of work was still required to develop better and more adaptable models and application programs of various pulping processes for computerized control. It was shown in earlier studies that the economic return through improved regulatory control justified the use of a computer (10, 43, 98). This project is aimed towards a study of some of the underlying principles and problems encountered in the area and the

reasons for choosing this particular topic are given in the following paragraphs.

The digester is at the front end of all pulp and paper mill unit operations (Figure 1.1) and therefore is a logical place to start a pulp and paper mill project. The pulp from the digester is utilized by most of the other sections and this affects the performance and production capabilities of all downstream units right down to the paper machine, which makes close control of the digester all the more important. It is a reasonably complicated chemical engineering process that involves complex physical and chemical relationships. There are also strong interactions between the manipulated variables, and the digester produces pure time delays and is therefore all the more difficult to control. Operating and output variables, like the alkali and wood component concentrations are unavailable or unmeasurable throughout most of the digester, and hence the system appears very much like a 'black box'. A systematic investigation of the digester should lead to better control by the computer.

A continuous digester was selected due to its advantages over a batch digester. The continuous digester

is at a disadvantage when production flexibility is required, but less equipment and energy is needed for the same production rate. Nowadays with environmental standards getting stricter, a continuous digester performs better here also because of the relative flow rates involved. It is estimated that a 500 air-dry-tons (ADT)/ day Kamyr continuous digester uses 124,000 fewer barrels of fuel oil per year when compared to a batch digester/drum washer system (51). The pretreatment of chips in the digester feed system gives improved liquor penetration and the high heat washing zone reduces the load on downstream washers. This makes it possible for closer control and these days the trend is definitely towards continuous digesters (51).

Kraft pulping of wood was chosen as it is the most dominant in chemical pulping. In 1974, 38% of the total pulpwood and 86% of wood residue used for pulping in Canada was for Kraft pulping, this is equivalent to 56% of the total production (92). In Sweden, which like Canada is one of the major pulp and paper producers, 59% of all pulp produced in 1973 was by the Kraft process (24 p134). Kleppe (59) has a table for 1969 that includes wood pulped in the United States and it shows a similar breakdown.

1.1 Wood

Wood is the principal raw material in pulp and paper manufacture. It consists of fibres joined together by a cementing material and numerous minor components which vary with the wood species. The colourless fibres are carbohydrates that consist of relatively long chained cellulose (5000-10000 monomer units) and shorter chained hemicellulose (1000-2500 units). The coloured binding material is lignin. The hemicelluloses, which react more rapidly than the celluloses, are further classified as mannans and xylans, which are short forms for longer chemical names. The extraneous substances include terpenes, resins and phenols which are soluble in organic and inorganic solvents and broadly termed as extractives. The main objective in all pulping processes is to separate the wood fibres from one another with maximum possible yield and minimum loss of fibre strength. These processes vary from semi-mechanical pulping characterized by a high yield of pulp suitable for low strength products such as fiberboard, to comparatively low yield chemical pulping for fine papers.

A combination of mechanical grinding and chemical separation called semi-chemical are between these two extremes. In chemical pulping, the lignin is extracted to the desired degree by using either an alkaline or acidic digesting liquor.

1.2 Pulp and Paper Manufacture

In a typical bleached pulp and paper mill , Figure 1.1, there are six principal distinct steps:

i) Preparation of Raw Materials,

ii) Pulping,

iii) Bleaching,

iv) Pulp handling and or Stock preparation,

v) Paper production,

and vi) Recovery of chemicals.

Logs are stored in the millyard before debarking and chipping in the woodroom. The chips from storage are screened to remove abnormal sized chips and undesirable material and then moved to the digester where they are treated with cooking chemicals at high temperature and pressure to produce pulp. Pulp defibration takes place

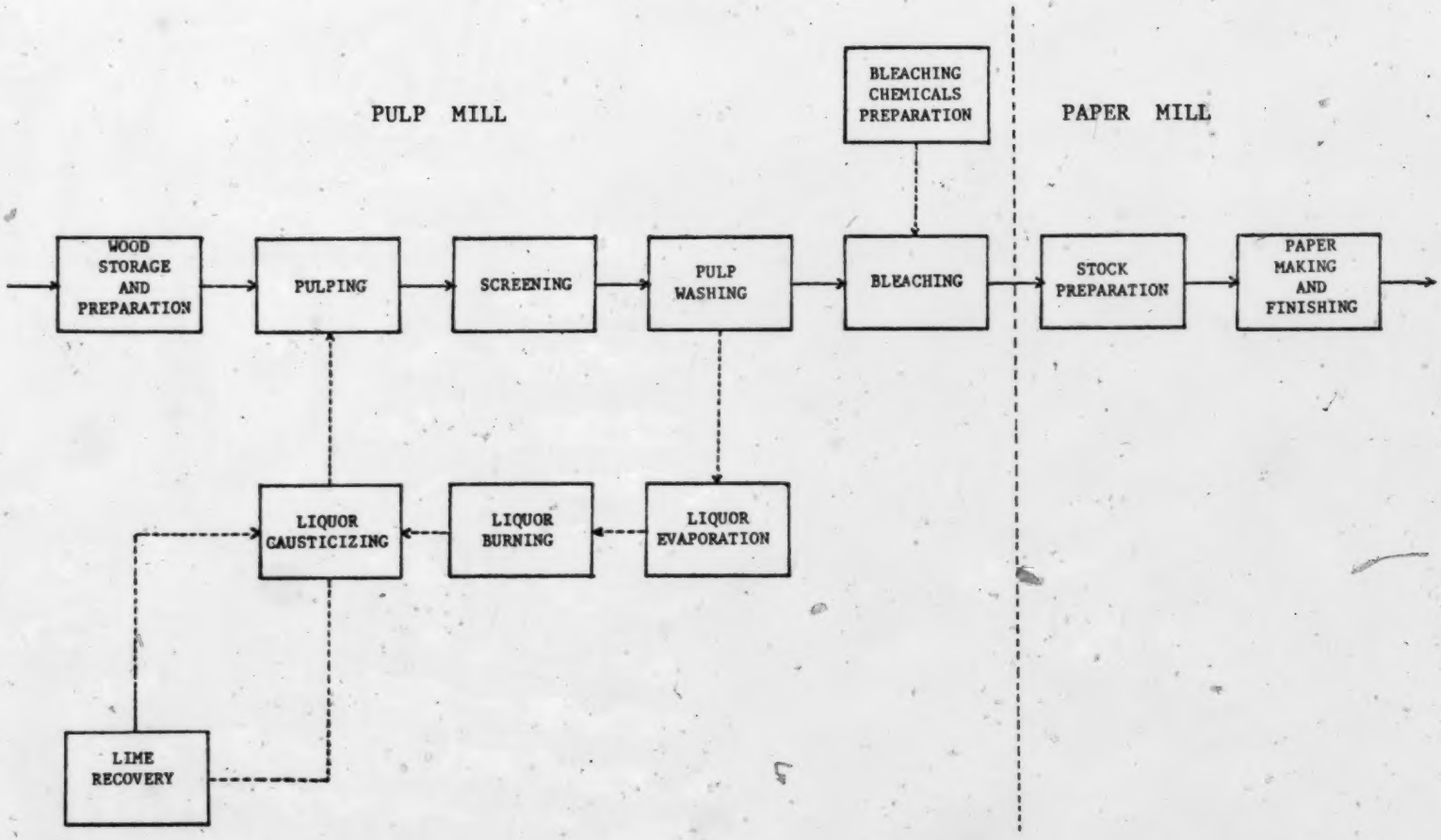


Figure 1.1 : Kraft Pulp and Paper Manufacturing Process

during the "blowing" of the digester. Pulp from the digester is then sent for screening operations in order to remove knots, bark fragments and uncooked material which are recycled back to the digester. The pulp is then pumped to the washers where spent chemicals are removed. Pulp washing is performed in the continuous digester, vacuum filters or in diffuser washers.

Washed, unbleached pulp is used for kraft linerboard and bag paper whereas pulps that require a high degree of brightness are subjected to bleaching with various chemicals. The bleaching process consists of a number of stages of reactors and vacuum washers where the pulp is bleached to the required terminal brightness. Typical bleaching sequences are CEHD, CEDED, and CEHDED where C designates chlorination, E is for caustic extraction, H is for sodium hypochlorite action and D, Chlorine Dioxide treatment.

Before paper manufacture, the pulp passes through a stock preparation stage. This involves refining and addition of chemicals. The refining includes beating of the pulp whereby the wood fibres are completely separated and chemicals are added to impart desired properties to the

paper sheet. The pulp slurry is then passed through the headbox onto a mesh screen to remove excess water. The resultant fibre mat is then pressed between heated rollers and dried. Finishing operations are next and the paper is coated, cut to size, rolled, weighed and moved to the warehouse for shipment.

Except for some small amounts of chemicals that are not recoverable in the washing stages, the major part of the chemicals used in the digesters are recovered and returned to the process. In the kraft process up to 99% of the cooking chemicals can be recovered. The spent chemicals or the black liquor is evaporated so that the resultant mass which has a chemical content of 60-65% can be burnt in the recovery boiler. The smelt from the boiler, after being dissolved in water , called the green liquor, is recausticized with lime to make fresh cooking liquor or white liquor.

1.3 Kamyr Digester

The Kamyr digester, Figure 1.2, is a hollow, cylindrical vertical shell where wood chips and the cooking chemicals, sodium hydroxide and sodium sulphide react continuously to produce pulp. The chips from storage are conveyed into the chip bin and then into a hopper which feeds the pockets of a rotating chipmeter that regulates flow into the digester. Chips leaving the meter are pretreated in the steaming vessel before falling through the chip chute into the high pressure feeder that sends them to the top of the digester. In the initial stages the chips absorb the cooking liquor without much reaction but as they travel further down the digester the temperature is increased by external heating in two steps. This is done by withdrawing the cooking liquor through cylindrical screens in the digester periphery and passing it through heat exchangers before returning it into the center of the digester, slightly above the screens. At a temperature of about 150 °C the rate of pulping increases considerably. The cooking time at this temperature depends on the product

specifications, usually the yield and the Kappa Number, and the production rate. The Kappa Number and sometimes the Permanganate Number are used as different measures of residual lignin in the pulp. The cooked chips are then quenched by injection of cool liquor to stop the reaction and the spent liquor is removed at the extraction screens below. This rate of liquor removal is larger than the flowrate in the cooking stage and thus results in a countercurrent flow of dilute liquor in the wash zone lower down in the digester. The spent liquor is sent to the flash tanks and evaporators for recovery. The countercurrent flowing liquor to the pulp acts as a washing medium and removes reaction products and unreacted chemicals from it. Near the bottom of the digester the wash liquor is heated externally to improve washing efficiency. The pulp is then cooled at the bottom and discharged through the outlet device and blow unit to the blow tank. It is then sent for further washing, and bleaching if so required.

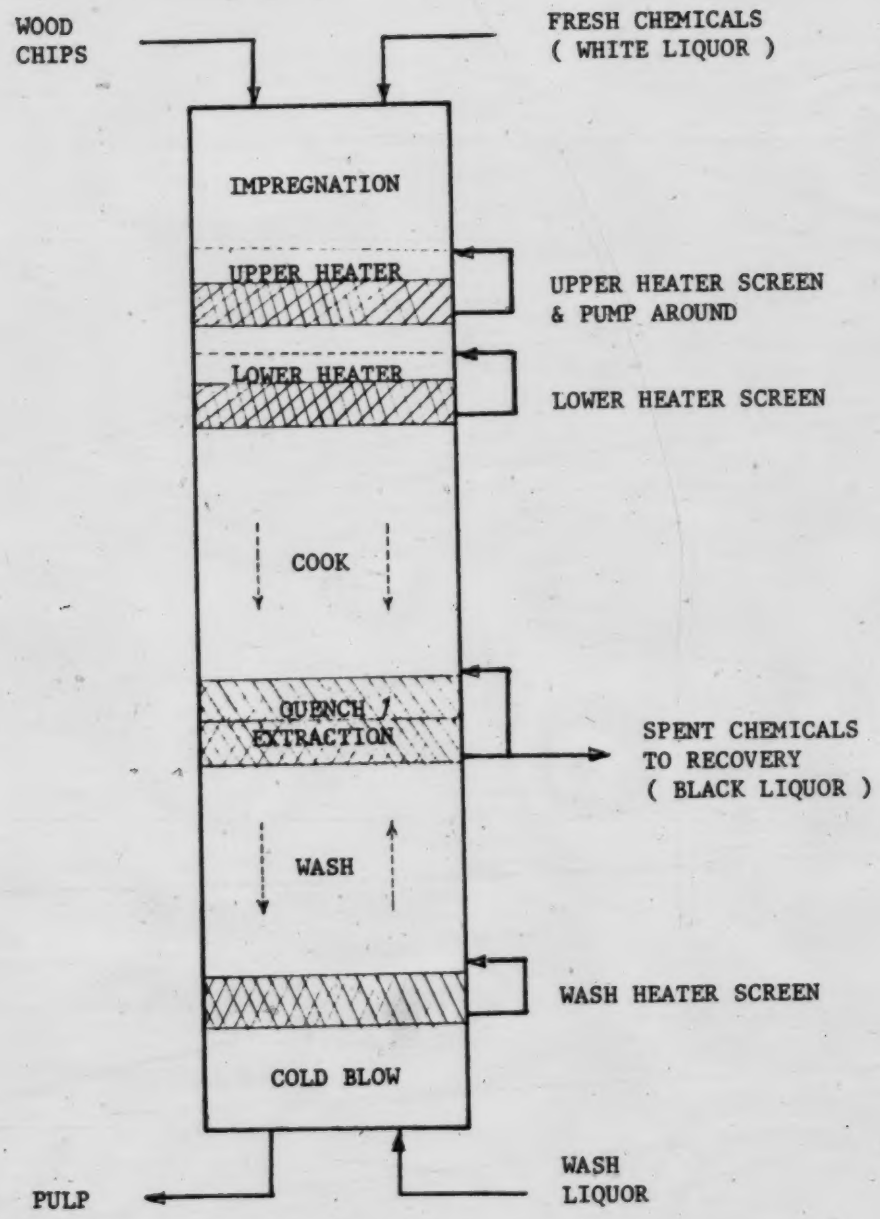


Figure 1.2 : Simplified Kamyr Digester Diagram

1.4 Objectives of Study

The objectives of this study were to document the state of the art and current operational practices for a Kamyr continuous digester and to derive a mathematical model based on the information available. This model was to be used to check out various open loop schemes and to work out a method for improving digester control . Part of the work was directed towards evaluating schemes such as "profile control", and multivariable computer control techniques that have worked well in other applications at the University of Alberta. It was hoped that simulation studies would suggest an improved control scheme for the Kamyr digester.

CHAPTER TWO

DIGESTER LITERATURE REVIEW

Alkaline pulping has been in prominence for nearly a hundred years now (59, 81 p279) and during this period investigators have tried to explain the reaction mechanism involved in wood pulping and derive applicable kinetic models. A number of review papers have been published on this subject in recent years. The Institute of Paper Chemistry has published a yearly review of progress in different aspects of alkaline pulping from 1947 to 1968 (46). Other papers by Wilder and Daleski (101) and Kleppe (59) provide information up to the time of publication. The textbooks on pulping processes by Rydholm (81) and "Pulp and Paper Manufacture" (70) have an extensive list of references also.

2.1 Review of Continuous Digesters

The first Kamyr digester was installed in Sweden in 1949 and the first in North America at Hinton, Alberta eight years later. Smith and McCorry (89) gave a description and operating procedures for the Hinton digester. Later changes and modifications in the digester cooking system are discussed in chronological order by Jansson (47), starting from the hot blow of pulp to the cold blow, diffusion extraction and high heat diffusion washing. Knutsson and Stockman (60) and McKibbins (74) provide evidence to support the improvement due to these innovations. Other types of continuous digesters are the steam phase digester, a two vessel high yield system with a separate pre-impregnation vessel and the saw dust digester with internal washing but the emphasis in this chapter will be on the conventional Kamyr hydraulic digester.

The continuous cooking process is also described in various texts and articles (12, 49, 70, 85, 88, 93) and an operating manual on this digester is published by the Scott Paper Company and distributed by Kamyr Inc (85). Hubbe

(43), in the first of a series of papers on digester computer control also gives a detailed description of the process. He includes a set of cooking variables and heat and material balances for two wood species, a hardwood and a softwood at four different production rates.

2.2 Digester Modelling Studies

Continuous digesters have been modelled with various degrees of complexity by researchers and computer vendors. Westinghouse installed one of the first digester computer systems at Gulf States Paper Corporation (28) but most of the modelling information was proprietary and not disclosed. Smith (90) has discussed the installation and and basic formulation of this model. Johnson (48) derived a linear model that is conceptually the same as that at Gulf States though it has less detail. He developed control equations using statistical regression methods for Kappa Number with cooking temperature and chemical concentrations as the dependent variables. His analysis was based on batch cooking data augumented with random noise. Similar

statistical work has also been done by Hoag (40), McKibbins et al (75), Hatton (36, 37) and Kerr (52, 53) and empirical equations developed relating the important digester cooking variables. Tucker (98) in a feasibility study for process computer control mentions a related model to the earlier ones for quality control and also includes a measure of the time delays involved. Later more exhaustive work based on chemical engineering principles was done by Stillman (93), Johnsson (49) and Smith and Williams (88) and will be discussed in more detail in the next section.

The digester wash zone has been modelled separately by Williams et al (103) as a distributed parameter system and steady state analytical solutions at various flow rates are given. Separate washing studies have also been done and a dynamic model which includes cooking in the wash zone has been presented by Wetlessen (100). A review of washing literature and a survey of countercurrent pulp washing theory and models has been presented by Toniak and Lauzon (96, 97). They have an extensive list of references and have presented the three basic models used in countercurrent washing theory. These models are all essentially a variation of perfect mixing cells in series with the washing

liquid and pulp flowing in opposite directions to each other.

2.3 Survey of Past Modelling Work

The major digester models developed by Stillman, Johnsson and Smith are discussed in detail and compared in this section. Table 1 summarises the assumptions and main features of each model.

2.3.1 Stillman's Model (93)

Stillman's work consists of two parts. A batch digester model was derived first to test the cooking model and then this kinetic model was used to derive a steady state model for the continuous case. The batch or cooking model consists of first order kinetic rate expressions that were derived from the literature existing at the time. Seven wood components were considered, for the broad classification or hardwood and softwood species namely, lignin, cellulose, mannan, xylan, acetyl groups, uronic acid and extractives. The reaction rate constants were derived

from laboratory cooking data and these constants include the effect of temperature via Arrhenius type relationships, and the effect of varying chemical concentrations in the cooking liquor . A sodium sulphide hydrolysis equation is used to calculate the amount of alkali instead of assuming fifty percent hydrolysis to the hydroxide and a factor for evaluating the effective sodium sulphide-carbonydrate reaction was developed after fitting cooking data. A liquor density relationship is also derived based on the expansion of water with temperature. The batch model so derived was tested against published results of hardwood and softwood cooks. The results compared fairly well, especially in the final stages of the cook.

While deriving the kinetic constants, Stillman mentions that although substantial literature existed on kraft pulping it could not be fully utilised because of the manner in which it was collected. The main problems were as a result of low liquor to wood ratios, insufficient cooking liquor pre-impregnation and unavailability of liquor concentrations during the cook and time to reach the maximum temperature.

The continuous digester model consists of a series

of axial sections. Steady state material and energy balances are conducted on each section where wood chips and cooking liquor are assumed to flow with the same velocity. Most of the equations derived for the batch model are used and an energy balance equation was the only extra one derived. The cooking equations are solved over the residence time of the pulp in each of the axial digester sections instead of the cooking time as was done in the batch model. The model testing results are not published as customer supplied data was used but sample calculations for total yield based on Hubbe's (43) data seem to agree well.

A comparison of one and two temperature cooks was made and a higher yield claimed for the same lignin content in the two temperature cook. A two temperature cook is where a high cooking temperature is followed by a lower one for the remaining portion of the cook, as opposed to a higher temperature in the latter portion of conventional continuous cooks. The detrimental effects of a chip moisture disturbance on pulp production rate and product quality were also studied by simulation from this model.

2.3.2 Johnsson's Model (49)

This model has two parts to it alsc. The first is a detailed distributed parameter model for all sections in the digester starting from the steaming vessel to the digester outlet valve. This model includes diffusion of chemicals and reaction products into the wood chip and involves a measure of chip thickness distributions. The second part is where the former dynamic model is simplified to a steady state one. In this static model, the wash zone is further simplified because of its countercurrent flow.

Mass and energy balances are derived for the wood and free flowing liquor. The wood is considered to have four constituents, lignin, carbohydrates, non extractable solids and easily extractable solids like acetyls and resins. The free liquor flows in the chip voids and the chemical concentration is assumed to be the hydroxide effective alkali alone since the effect of bisulphide concentration is neglected. Effective alkali is defined as the total sodium hydroxide concentration, assuming that fifty percent of the sodium sulphide (Na_2S) is hydrolysed to

sodium hydroxide (NaOH) and is expressed in terms of sodium oxide (Na_2O). Reaction kinetics in the model are first order in lignin and the carbohydrates are monitored by a lignin-yield functional relationship, that is assumed known for the particular wood species.

Partial differential equations for the model are derived with lignin, carbohydrates, yield, reaction products and effective alkali as the dependent variables. These equations are similar in form in the top half zones of the digester with the cocurrent flow, as the only difference is with respect to the section's temperature. The temperature profile and residence time relationship are assumed known and specified. The external heater streams are assumed to be perfectly mixed with the free liquor in the vicinity of the screens. Equations for the wash zone are derived from those for the cooking zone by neglecting the pulping reactions and reversing the sign of the appropriate flow terms to account for the countercurrent free flow of wash liquor. This simplifies the model to essentially include only the diffusion of chemicals and reaction products out of the cooked chips. Johnsson mentions that a model that includes cooking in the wash zone has also been derived but

was not included in the published work.

The dynamic model is reduced to a steady state model because of computational convenience and for testing and design purposes. Johnsson mentions that this static model is fine for design but not for control purposes. The static model includes the basic nonlinearities of the dynamic model, the same reaction kinetics, and the same dependence on temperature and chip thickness distribution. Some of the assumptions made to obtain a solution are a constant production rate, absence of disturbances in the input variables and wood parameters and a constant chip size distribution throughout the digester. The static wash zone problem is converted from a boundary value problem to an initial value one by parameter transformation.

The Johnsson model verification and testing was done using data from a high yield kraft mill digester operated at a higher and lower than normal production rate. The major discrepancies were between the observed and calculated Kappa numbers. This was attributed to the presence of cooking in the wash zone, errors in plant effective alkali measurements, diffusion coefficients and wood density values used and approximations in the model.

Several studies with parameter variation and disturbances in the input variables were tried. They include variations in temperature, lignin and acetyl content, liquor/wood ratio, alkalinity, rate coefficients, density change and the amount of void volume in the chip pack. The wash studies include the effect of washing variables, such as dilution factor or wash flow on washing efficiencies.

He concludes that alkalinity, liquor/wood ratio, temperature and cooking time affect the quality and cost of production of the pulp and that chip thickness distributions are helpful in studying pulp inhomogeneity and washing efficiency.

2.3.3 Smith and William's Model (88)

This is a dynamic model with a series of lumped, axial sections starting from the digester top to the exit. Each of the sections in the model is assumed to include three phases. Therefore a section is further divided into three subsections, the wood, the absorbed or entrapped liquor in the wood, and the cooking liquor between the chip voids that is free to move about and is termed the free

liquor. The model considers twelve state variables, five for the wood components, three each for the component concentrations in the free and the entrapped liquors, and the temperature of the section. The five wood components considered are fast and slow reacting lignin, and the three carbohydrate fractions, cellulose, mannan and xylan. The liquor component concentrations included are hydroxide effective alkali and bisulphide ions, from the hydrolysis of sodium sulphide and the reaction products. The temperature in the section is assumed to be identical in the three phases (the wood, entrapped and free liquors) except when an externally heated stream is introduced. The external heater stream is included in the free flowing liquor and complete mixing between the two is assumed. The dynamic mass and energy balance equations derived for each of the sections assume that it is an ideal stirred tank reactor so that the exit streams have the same conditions as that in the section. They claim that the kinetic model that was developed is based on observed chemical principles. Reaction rate constants are developed from laboratory and industrial data for various hardwood and softwood species. Other assumptions made in deriving the model are that the

entering and exit flows occur in their respective phases and subsections and that there is no accumulation of wood and entrapped liquor, this gives constant flow rates to the wood and entrapped liquor and consequently the same velocity and residence time. The residence time data used was taken from Johnsson (49), who has presented a curve for chip volume fed versus digester elevation. The free liquor rates are constant also, except where there are external flows and in that case they are taken as the sum total of both flows. The mass transfer rate between the entrapped and free liquors is proportional to the concentration difference between the two phases and the rate coefficients are assumed to be identical for all the components. The mass transfer coefficients have a temperature dependence and piecewise curves were fitted to data derived from the Chilton Colburn analogy.

The wash zone model is simplified by neglecting the cooking reaction and considering only the dissolved solid concentration and the temperature. This reduces the number of state variables in the model to three. Dissolved solids or reaction product concentrations in the entrapped and free liquors and the section temperatures were calculated for

different wash flows and the results plotted as washing efficiency and wash flow rate. Clean wash water studies were done also and a comparison made with those using dilute liquor. They conclude that clean water washes are more economical than the conventional dilute liquor washes, since better washing efficiencies for the same flow are obtained and thus save energy and evaporation costs.

Testing of the Smith model was done with actual industrial data and the results agreed fairly well. The kinetic model results had deviations from actual laboratory data in some cases, but this is termed to be the best possible fit. Dynamic simulations were done by varying the chip moisture, alkali content, the lower heater temperature, and flow stoppage in the digester. All the results are as would be expected. However the working of the model is such that to simulate a flow stoppage from the blow line the chipmeter speed has to be set to zero. The wash zone results had substantial disagreement with those from Johnsson (49). They state that though the differences between the results are large, the magnitude of error is the same for all cases. This discrepency is probably due to inaccuracies in the mass transfer portion of the model.

CHAPTER THREE

DERIVATION OF MODEL

This chapter on the Kamyr digester model starts with a detailed description of the digester and the accompanying equipment with typical operating conditions. This is followed by the details of a digester section that is representative of all its zones. The assumptions made for deriving the model and the reasons for their choice are discussed next. Then a review of the kinetic literature, the derivation of model kinetics, and the batch or cooking model are presented. The chapter ends with reasons for choosing the particular model. A comparison of Kamyr digester models and assumptions from Stillman (93), Johnsson (49) and Smith and Williams (88) and this work are given in Table 1.

3.1 Detailed Digester Description

There are six distinct processing stages that wood chips have to pass through in a continuous digester system,

namely: presteaming and conditioning, cooking liquor impregnation, heating of chips and liquor, cooking of chips, washing of chemicals and reaction products, and cooling before the pulp leaves the digester. A detailed piping and instrumentation diagram for the digester is given in Figure 3.1.

Chips are moved from the chip bin to the hopper that feeds the rotating chipmeter. The chipmeter rotor speed is set to a given digester wood feed rate and the low pressure feeder then introduces the chips into one end of the cylindrical presteaming vessel. Here, they are slowly conveyed by a rotating screw to the discharge end. The vessel operates at 15 to 20 psi and 65 $^{\circ}$C (150 $^{\circ}$F). Retention time and temperature are limited to prevent prehydrolysis of the hemicelluloses for this would limit the yield and the pulp beating and strength properties. The presteaming and conditioning stage thus accomplishes removal of non-condensible gases and terpenes, the terpenes are separated later and represent a valuable byproduct. It also raises the temperature and moisture content of chips which facilitates liquor impregnation and increases the density so that the chips will sink more readily into the digester

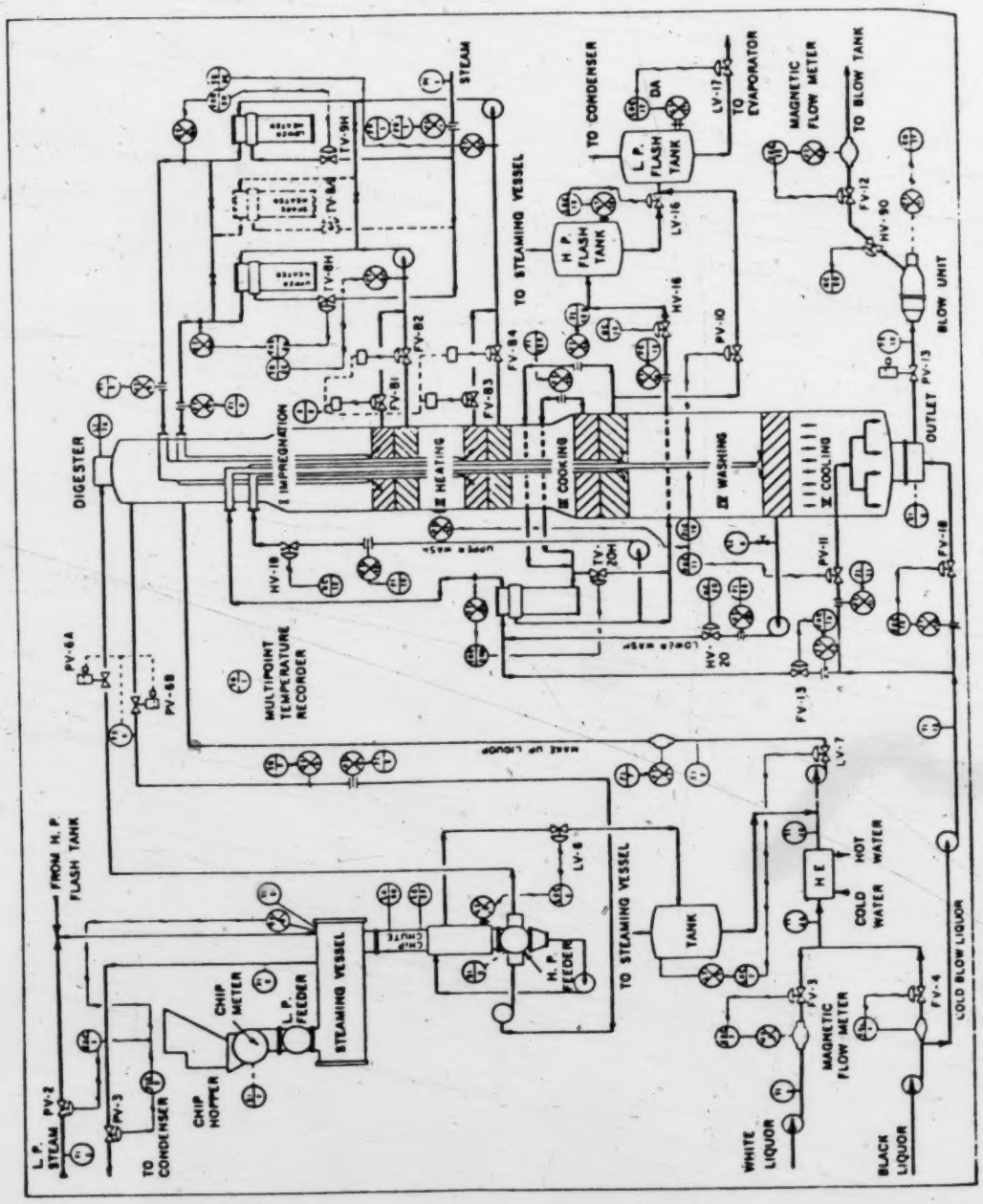


Figure 3.1 : Kamyr Digester Process Diagram (Lavigne (57))

cooking liquor.

Upon discharge from the steaming vessel, The chips fall into the chip chute which is partially filled with liquor and impregnation begins at this time. The liquor level of the latter is held constant by a controller. Below the chip chute is a rotary type high pressure feeder and the chips are transfered from a pressure of 15 psi to the pressure at the digester top of 165 psi. Chips and liquor enter one of the exposed feeder pockets which are so placed that there is at least one pocket in receiving and another in discharging position. The chips in the pocket are retained while the liquor drains to the intake of the chip chute circulation pump. The chips are flushed out as the pocket gets to a horizontal position by liquor from the high pressure top circulation pump and conveyed to the top separator in the digester. The top separator is a helical screw surrounded by a cylindrical screen that separates the liquor, which is returned to the top separator circulation pump intake as the chips pass into the digester impregnation zone. The makeup cooking liquor is introduced below the top separator and consists of white and black liquors in the correct alkali to wood (A/W) and liquor to wood (L/W)

ratios.

In the impregnation zone the chips rapidly absorb liquor as they move downwards by gravity. It is important that the chips be throughly impregnated for if impregnation is incomplete, the chips would be left with uncooked centers. Normally the chips spend 45 minutes at temperatures ranging from 100 to 125 °C (215 to 260 °F). The cooking reaction is negligible at these temperatures and the sole purpose is diffusion of active alkali into the chips.

The chips are now ready for cooking and their temperature is raised to 150 °C (305 °F) in the upper heater zone. Hot liquor enters the center of the digester from the outermost of the concentric pipes and moves radially outwards to the screens in the periphery of the digester. There are two screens but only one of them is extracting at a time. This is to allow the descending chip mass to remove the chips that are adhering to the screen slots from the preceding operating period. The switching of screens is accomplished by a time switch that opens control valves on the liquor lines alternatively. The same operation is repeated lower down in the lower heating zone and the

temperature is raised from 150 °C to 165 °C (330 °F).

The chips next move through the cooking zone where actual cooking of chips takes place. The active chemicals in the cooking liquor, sodium hydroxide (NaCH) and sodium sulphide (Na_2S) react with the lignin and convert it into compounds which dissolve in the cooking liquor. The liquor also attacks the carbohydrates, which is undesirable for this reduces the yield and alters the pulp characteristics. Cooking time is therefore selected to obtain the desired yield, pulp qualities and production rate. A typical time is about 90 minutes.

During passage through the cook zone the pulp temperature rises by up to ten degrees as the pulping reactions are exothermic. The pulp is then quenched by injecting cool liquor. The temperature of quench liquor has a marked effect on the reaction rate and if the pulp quality is not suitable then the cooking time is extended by allowing cooking to continue into the wash zone. At the third set of screens, the extraction screens, the quench liquor displaces the spent cooking liquor through the upper screen. The spent liquor flows to the flash tanks where steam is produced for the steaming vessel. Liquor is then

sent to the evaporators for recovery. The lower screen extracts dilute black liquor from the washing zone, in the lower part of the digester. The majority of this liquor is used for quenching and the rest is mixed with the extraction flow from the top screen and passes to recovery. The quench temperature is sometimes independently adjusted by mixing with a cold liquor stream termed "cheater" flow.

The chips continue downward and the countercurrent flow of wash liquor removes chemicals and dissolved solids from the chips by displacement and diffusion. This liquor is introduced at the bottom of the digester and is heated to about 135 °C (275 °F) in the wash heater near the bottom. This is done to improve the rate of diffusion and washing efficiency in the zone and is termed "Hi-heat" washing, as the temperature is higher than that of the vacuum drum washers. Residence time in the zone varies from 60 to 240 minutes depending on mill requirements and downstream washing facilities.

In the cold blow zone, the cooked chips are cooled to 70 to 94 °C (160 to 200 °F) by injection of wash liquor at 60 to 82 °C (140 to 180 °F) in the bottom of the digester shell. It is this liquor that is heated up to form the wash

liquor in the preceding zone. The cooled chips are then removed from the digester by the outlet device. The chips have to be cooled for if removed at the cooking temperature sudden expansion and mechanical action results in loss of pulp strength. The outlet device rotates at a speed of 3 to 16 rpm. The speed is adjusted to meet internal digester conditions such as the blowing rate and desired pulp consistency. The chips at a pressure of 200 psi are removed in three stages of pressure drop through the blow unit to the blow tank or storage.

3.2 Description of a Digester Section

For purposes of modelling, the digester's seven zones are split up into ideal stirred tanks or lumped parameter sections of uniform temperature and composition. These sections are not necessarily of equal volume as they are divided to match the digester configuration and for computational convenience.

A digester section is further subdivided into sub-sections to represent the three phases, oven dry wood, the entrapped or absorbed liquor in the wood and the free

liquor flowing in the void volume. The wood and the entrapped liquor are in temperature equilibrium but the free liquor has a temperature of its own, as external flows to the digester mix only with the free liquor. In the wash zone this liquor flows countercurrent to the chip mass.

For material and energy balances thirteen state variables are considered: Wood flow in mass of oven dry wood/minute; four wood components, lignin, cellulose, mannan and xylan as mass fraction percentages of oven dry wood; the temperatures of the wood and free liquor; and three concentrations each for the entrapped and free liquors, sodium hydroxide, sodium sulphide and reaction products.

3.3 Model Assumptions

The assumptions made for deriving the model are presented and their reasons are given.

3.3.1 Steaming Vessel

i) The temperature of chips and the enclosed moisture is raised to that of saturated steam in the steaming vessel. This is based on condensation of steam

with no steam losses.

Mathematically,

$$Wcond * Hcond = (Ww * Cpw + Wmo * Cpm) * (Tsv - Tw)$$

where

Wcond is the mass flow of steaming vessel condensate,
Hcond is the latent heat of condensing steam,
Ww is the mass flow rate for wood chips,
Wmo is the mass flow of moisture in the wood chips,
Cpw and Cpm are the specific heat of the wood and moisture,
Tsv is the steaming vessel temperature
and Tw is the temperature of the chips.

ii) Moisture in excess of the fibre saturation point freezes when temperatures are below the freezing point. The fibre saturation point is reached at about 30% moisture content.

The first assumption is made so that the steam condensate that flows along with the chips and dilutes the liquor can be estimated. This is reasonable as past experience in industry has shown (27). The second

assumption has been found experimentally by Stone and Scallan (95).

3.3.2 A Digester Section

i) Each digester sub-section is assumed to be an ideal stirred tank, i.e. it is perfectly mixed.

ii) The wood is assumed to consist of lignin, cellulose, mannan and xylan. There are also some easily removable components, such as, uronic acid, acetyl groups and extractives.

iii) The bone dry wood substance density is constant at 1.53 (95.5 lb/ cu ft) and there is little variation with species, composition or type of growth.

iv) The chip movement is by plug flow and the velocity is a known function of distance from the digester top, geometry, pulp density and withdrawal rate.

v) The chips undergo compaction as they move down

the digester, i.e., their bulk density increases.

vi) Entrapped liquor volume is based on the critical moisture content of the chips.

vii) Digester liquor consists of sodium hydroxide, sodium sulphide and reaction products termed 'dissolved solids'.

viii) The downward movement of liquor in the cooking sections is plug flow and the residence time of both the entrapped and free liquors is assumed to be the same as the wood.

ix) No back mixing of materials between sections is assumed.

x) Sodium sulphide hydrolysis is based on an empirical relationship between the liquor component concentrations and the temperature.

xi) All the reaction products are converted to

dissolved solids and the pulp yield is a sum of the wood component concentrations.

xii) Heat exchange with the digester walls is divided proportionately between the wood and entrapped liquor and the free liquor.

xiii) Entrapped and free liquor flow in their respective sections with their own temperature and heat transfer between them depends on their temperature difference.

xiv) The liquor and wood specific heats and heat transfer coefficients are independent of temperature as average values in the operating temperature range are used.

xv) The mass transfer coefficients are equal for the three liquor components.

xvi) There is no mass transfer of wood components by diffusion.

The continuous digester is a tubular reactor which

can be represented by N stirred tanks, especially when N is large. So assumption (i) is reasonable. The basis for (ii) is that the major wood constituents are lignin, mannan, xylan and cellulose and the easily removable components dissolve in the early part of the cook. The density of wood substance, assumption (iii), is from actual experimental data by Stamm and Hansen (91).

The residence time data ((iv)) was presented by Hamilton (34) and Johnsson (49) from radioactive tracer studies on a continuous digester. The chip velocity is observed to decreases down the digester and this is due to chip compaction ((v)).

The volume of the entrapped liquor ((vi)) in the chips is a function of liquor density, as the chips swell up and reach the critical moisture content limit which is known.

Digester liquor composition ((vii)) is mainly sodium hydroxide, sodium sulphide and reaction products, although chemicals such as carbonates, sulphates and other sulphides are formed in the recovery cycle they are either negligible or inert to the pulping reaction.

Plug flow for liquor ((viii)) and negligible radial

gradients or backmixing ((ix)) are assumed to simplify the mathematical model. There is also no backmixing of the chips (34).

The sodium sulphide hydrolysis ((x)) is from Martin (72) and the actual relation used is taken from Stillman (93).

Assumption ((xi)) on yield and reaction products follow from a mass balance on wood. Since the wood concentrations are mass fractions on a percent oven dry wood basis, a sum of the individual concentra tions would give the percentage yield.

Assumptions ((xii)-(xiii)) are made to simplify the heat exchange model between the wood, free and the entrapped liquors. The temperature difference between the wood plus entrapped liquor and the free liquor is due to the effect of an external heater flow, which mixes with only the free liquor. It takes the wood and entrapped liquor some time to reach that temperature.

The liquor and wood heat transfer coefficients are taken to be constant ((xiv)), as data was not available for their variation with temperature. The wood specific heat relationship with temperature has been studied by Dunlap

(22) and an average value in the digester operating range is used in the model. The liquor specific heat value was similarly determined. The assumption for diffusion of wood component ((xvi)) being neglected is because the transport of pure substances by the flow of wood and liquor is much larger than that by diffusion.

3.3.3 Impregnation Zone

i) The flow of chips entering the first digester section is based on the chip meter flow and the blow flow leaving the digester, and

ii) The easily removable wood components are assumed to completely react in the impregnation zone.

The first assumption ((i)) for chip flow to the first section is apparent when a stoppage in chipmeter or blow flow is considered.

The easily removable wood components have a high reaction rate and it is observed that they are not present at the end of the cook. Simulation studies by Stillman (93), who considered no such assumption ((ii)) showed this to be true.

3.3.4 Heating Zone

i) Heater flows involve no mass transfer and only help to raise the free liquor temperature.

This assumption is to simplify calculations, since the external flow is a pump around stream and would have the component concentration equal to that in the digester section from which it is removed, at steady state.

3.3.5 Cooking Zone

i) Lignin, mannan and xylan have varying reaction rates, depending on their concentration and process conditions. These rates are termed extractive, bulk and residual and relate to the ease of removal of the wood components.

ii) The reaction rate for a wood component Z is of the first order type and can be written as:

$$\frac{dZn}{dt} = -kij*Zn$$

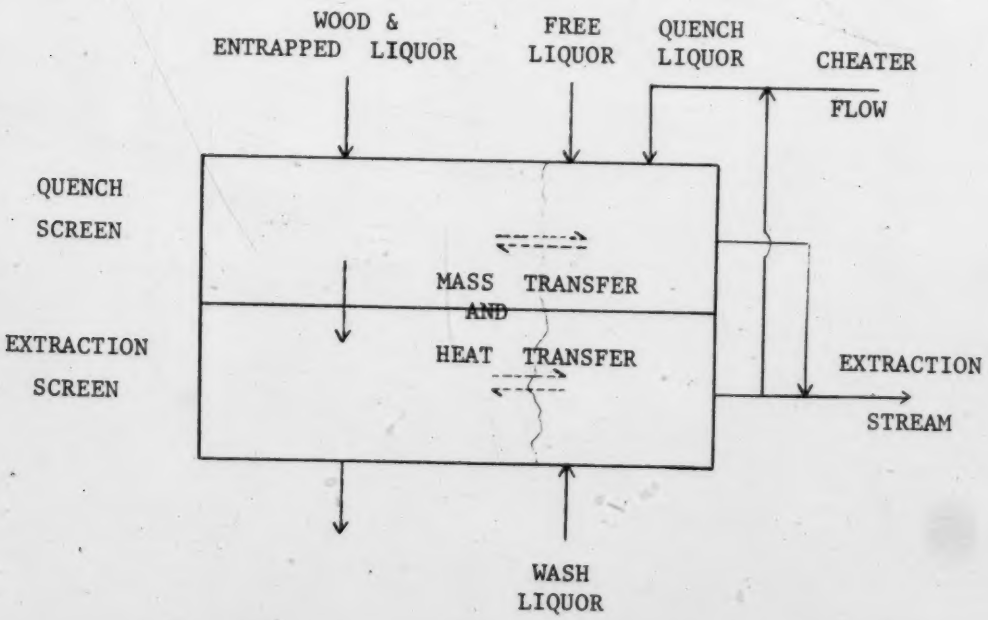
where Zn is the concentration of component Z in section n and kij is the reaction velocity constant that is dependent on the liquor concentrations and temperature.

iii) The reaction rate is dependent on the entrapped liquor concentration.

Assumptions (i) to (iii) and comments on them are presented in section 3.4 .

3.3.6 Extraction / Quench Zones

The extraction/quench screens with their complicated flow patterns are treated as a perfect mixing zone for free liquor, from the cooking and wash zones. The flow patterns assumed are shown below.



This assumption for perfectly mixed free liquor

streams follows from the earlier assumption for heater flows (3.3.2 (i)).

3.3.7 Washing Zone

Free liquor in the wash zone is countercurrent to the wood flow but there is considered to be no backmixing between sections. Plug flow is assumed.

This assumption is just an extension of 3.3.2 (viii), 3.3.2 (ix) and 3.3.2 (xvi).

Table 1 Comparison of Kamyr Digester Models

	STILLMAN	JOHNSSON	SMITH & WILLIAMS	THIS WORK
Models covered by study	Batch digester and steady state continuous digester models	Dynamic and steady state models of Kamyr digester	Batch and dynamic continuous digester models	Batch digester model, steady state and dynamic model of a Kamyr digester
Number of the dependent variables in continuous model (details below)	Ten variables, seven wood, two cooking liquor & temperature	Five variables, three wood and two for cooking liquor	Twelve variables five wood, six liquor component concentrations & temperature	Thirteen variables one for varying wood density, four wood components, six liquor and two for temperature
Number of zones considered in the digester model	Six: Impregnation, heating, cooking, quench, washing & cold blow	Four: Impregnation, heating, cooking & washing	Seven: Impregnation, upper & lower heating, cooking, quench, washing & cold blow	Eight: Impregnation, upper & lower heating, cooking, quench extraction, washing & cold blow
Number of phases in a digester section	Two phases: wood & cooking liquor	Two phases: chips & cooking liquor	Three phases: wood, entrapped liquor in wood & free liquor	Three phases: wood, entrapped and free liquor

... continued

Table 1 (continued)

	STILLMAN	JOHNSSON	SMITH & WILLIAMS	THIS WORK
Wood components considered	Seven: Lignin, Cellulose, Mannan, Xylan, Acetyls, Uronic Acid & Extractives	Three: Lignin, Carbohydrates, & fast reacting Acetyls & Extractives	Five: Fast & slow reacting Lignin, Cellulose, Mannan & Xylan	Four: Lignin, Cellulose, Mannan & Xylan
Liquor components and pulping agents	Sodium hydroxide (NaOH) & sodium sulphide (Na2S)	Effective alkali (NaOH+0.5*Na2S) and reaction products	Effective alkali bisulphide (HS-) and reaction products	Hydroxide, Sulphide (S--) and reaction products
Energy balance and temperature calculation	Steady state heat balance to give section temperature	Temperature profile is specified	Dynamic heat balance for equilibrium temerature of wood, entrapped & free liquor. Exception is with external heater flows	Two energy balance equations for wood & entrapped liquor; & free liquor. External heater mix with free liquor
Chip movement and residence time	Plug flow of chips. Residence time is a function of chip meter flow & compaction	Plug flow for chips. Residence time is known function of chip meter flow	Same plug flow & residence time relation as Johnsson	Plug flow. Residence time is a function of chipmeter & blow flows & compaction

... continued

Table 1 (continued)

	STILLMAN	JOHNSSON	SMITH & WILLIAMS	THIS WORK
Chip compaction	Constant values at points in digester, irrespective of rate of production	Function of digester position and chip volume fed at digester top	Same function as Johnsson	A function of position and degree of cooking (H-Factor)
Chip size	Standard chips	Effect of chip thickness included with diffusion into chip. Size distribution is constant	No effect of size as standard sized chips assumed	Normal chip size distribution is assumed which makes diffusion effects negligible
Rapid reacting wood components eg Acetyls	Three components & their reaction included	Assumed to react instantly	React instantaneously	Assumed to react completely in the impregnation zone
Pre-steaming and condensate flow	Condensate flow is read as input variable	Assumption from Fox (43). Includes frozen chips calculation	As in Fox	Fox's assumption: No heat losses in steaming vessel. Option for frozen chips. Condensate flow based on heat chips to saturated steam temperature

... continued

Table 1 (continued)

	STILLMAN	JOHNSSON	SMITH & WILLIAMS	THIS WORK
Mass transfer in the chips	None	Diffusion of chemicals & reaction solids in the chip. Coefficient is a function of temperature	Transfer of chemicals & reaction products between entrapped & free liquor related by temperature dependent mass transfer coefficient	Same as Smith & Williams
Carbohydrates in wood	Kinetics include carbohydrates as cellulose, mannan & xylan	Carbohydrates lumped together & concentration based on yield & lignin content	Included as Cellulose, Mannan & Xylan	Considered as Cellulose, Mannan & Xylan
Kinetic model	First order kinetics for wood components Rate constant is function of liquor component concentrations, wood component reaction rate phase and temperature. Eqn 3.4. (ii) & 3.4. (iii)	Reaction rate for lignin is first order. Rate constant is a product of effective alkali & constant ie k(T) *(OH-) *L	Kinetics are based on wood component concentration, effective alkali & & bisulphide concentration in in the form of Eqn 3.4. (v)	First order kinetic model similar to Stillman, with rate constant varying with wood component concentration, chemical concentration & temperature

... continued

Table 1 (continued)

	STILLMAN	JOHNSSON	SMITH & WILLIAMS	THIS WORK
Wash zone model	No reaction or washing zone calculations	No reaction in zone, though model with reaction exists	No reaction in zone. Has only temperature & dissolved solid concentration	Reaction & option with complete calculations provided
Numerical Computation	Analytical solution for first order equations is derived & soled over residence time of wood component in the digester section	Partial differential equations are solved in terms of axial & radial distance for a steady state profile. Solution technique not presented here	The fourth order Runge-Kutta method is used to to integrate the the set of ODEs	A fourth order Runge-Kutta Merson routine is used to generate a dynamic profile. Steady state model in same program but batch model is separate
Presentation of results	Digester history listing	Digester profile plots	Listing & plots for digester profiles	Listing & plots for digester profile & history

3.4 Model Kinetics

A literature survey and review of past kinetic models is presented, followed by the kinetic model used in this work and the reasons for its choice.

3.4.1 Literature Survey

The pulping reaction and its kinetics are very complex and have been studied by a number of researchers but there is still no general consensus on a single uniform model (59, 67, 101). Pulping is governed mainly by the rate of delignification and this reaction has been extensively examined. The undesirable side reactions, such as carbohydrate degradation cannot be avoided and have to be minimized so their kinetics have been of interest also.

Lignin occurs in amounts varying from 20 to 35% of the wood depending on the species. It is a large three dimensional polymer made up of phenyl-propane monomers that are linked together in various forms. A suggested reaction mechanism is at the solid-liquid interface by the hydroxide or sulphide (or hydrosulphide) ions present in the liquor

(59). These fragments dissolve as phenolate or carboxylate anions or they can undergo reactions with themselves , the undissolved lignin , or possibly also with the carbohydrates. The lignin that undergoes alkaline condensation reactions is more difficult to remove and so this reaction has to be prevented. There are indications that sulphide or hydrosulphide ions help in reducing these condensation reactions (59).

In most alkaline pulping the desired specifications are met by 50% lignin removal, but along with this 10 - 15% of the cellulose and at least 50% hemicellulose are removed. As mentioned earlier, the cellulose removal is undesirable for it results in approximately a 55% pulp yield based on an oven dry wood basis and is a very important economic factor as the cost of wood is a major part of the total production cost of pulp. For this reason efforts have been made to minimize the carbohydrate reaction and enhance the yield. In the early stages of the cook, hemicelluloses are reduced by 40% while the lignin dissolved is just 20% (59). The introduction of certain additives such as anthraquinone to the pulping liquor look promising in reducing the carbohydrate reaction. Recently patents have been issued

for methods of reprecipitating the hemicelluloses that is dissolved in the earlier stages of the cook (46).

The carbohydrates consist of basic linear polymers made up of glucose (cellulose), xylose (xylans) and a copolymer of glucose and mannose (glucomannans and galactoglucomannans). The carbohydrate polymer degradation process is dependent on polymer size or degree of polymerization and the accessibility to pulping liquor. There are predominantly three basic types of reactions. The first is the "peeling" reaction, which causes the bulk of the yield loss, and is the removal of the reducing end groups from the polymer. After an end group has been removed, the remaining end group can again be removed by "peeling" or can be stabilized by conversion to an acid group. This is the second type and is referred to as the "stopping" reaction. Chemically the "peeling" reaction relates to the free carbonyl groups which are not stable in alkali and split up with about sixty monomer end groups as iso-saccharinic acids. In the "stopping" reaction the molecule is stabilized by formation of meta-saccharinic acid end groups. The third reaction class is "random cleavage" of the molecule. This occurs at temperatures of above 150 C

with random alkaline hydrolysis of accessible glucosidic linkages. This exerts a dual effect in the loss of yield for small alkali soluble polymers are created and also new carbonyl end groups are formed where further "peeling" reactions can occur.

Overall, glucomannans and hardwood xylans are especially susceptible to the "peeling" reaction. The former is the main hemicellulosic component in softwoods and the latter in hardwoods. Softwood xylans are relatively stable and only 25 - 30% of them are removed in normal kraft pulping (59). Several theories exist but it is not known why this is so (70 p431, 81 p604).

The next important pulping variable is the liquor composition. Normal kraft liquor is made up of an aqueous solution of sodium hydroxide and sodium sulphide where the sodium sulphide is introduced as sodium sulphate in the chemical recovery cycle. This is due to the faster lignin reaction rate observed with the addition of sodium sulphide.

The kraft liquor components have the following equilibria (101) :

$$NaOH \rightleftharpoons (Na^+) + (OH^-) \quad (i)$$

$$Na_2S \rightleftharpoons 2(Na^+) + (S^{2-}) \quad (ii)$$

$$(S^{2-}) + H_2O \rightleftharpoons (OH^-) + (HS^-) \quad (iii)$$

$$NaSH \rightleftharpoons (Na^+) + (HS^-) \quad (iv)$$

$$(HS^-) + H_2O \rightleftharpoons (OH^-) + H_2S \quad (v)$$

Liquor concentration definitions involve these equilibrium concepts. The <u>active</u> alkali definition assumes reactions (iii) and (v) are complete which means that the hydroxide ion concentration is a sum of the sodium hydroxide and sodium sulphide molar concentrations. While the <u>effective</u> alkali definition assumes that reaction (iii) is complete and that reaction (v) is insignificant. The alkali concentration is then a sum of the sodium hydroxide and half that of the sodium sulphide.

It is difficult to determine the exact hydroxide, sulphide or bisulphide equilibria involved especially the effect of the individual contribution of sulphur ions towards pulping (101), but consistent pulping results are

obtained if the effective alkali concept is used as opposed to that of the active alkali.

3.4.2 Review of Kinetic Models

The overall pulping reaction involves five steps which proceed in sequence. If one step is slow compared to the others then it is said to control the overall rate. These steps, with respect to pulping are movement of reactants or chemicals into the chips, adsorption of chemicals onto active sites, the actual chemical reaction, desorption of reaction products and transport of desorbed reaction products out of the chip. The first and the fifth transport steps involving the transport of chemicals and reaction products become more prominent as the distance from the chip surface increases. This was observed from studies on chip thickness and shape on pulping rate. Backman (3), Hartler and Ostberg (35), Larocque and Maass (63) and Kulkarni and Nolan (61) conducted such experiments and found that the thickness was important above a certain "critical value" which varied with the cooking temperature. This critical thickness has been assigned varying values of 1 mm

(3), 3 mm (35) and up to 10 mm (63) but the effects of diffusion can be minimised if a chip with a thickness of 2 to 3 mm or less is used with current digester pulping temperatures (101). The same observations are obtained when the reaction rate coefficient of 30 Kcals/mole (21) is compared with that of diffusion limited processes at 5 - 6 Kcal/mole (81 p309). For soda pulping, Daleski (21) suggests 195 ^{o}C as the temperature above which diffusion becomes dominant. Liquor diffusion is important in impregnation (81 p265) and additional methods of forced penetration by liquor and gas flow or high pressure impregnation have been developed to achieve uniform impregnation and thereby uniform pulping with minimum amount pulp rejects. The effects of diffusion on pulping were also studied by Johnsson (49) using computer simulation and varying chip thickness distribution, penetration depth and diffusion coefficients, and similar results on pulping and rejects were obtained.

The chemical reaction step involves two dissimilar phases, wood and liquor which gives a heterogeneous reaction system. This is extremely difficult to evaluate and so homogeneous models have been generally derived

mathematically in terms of a rate expression and from analysis of actual cooking data. Several models have been developed on this basis and the effects of liquor composition and temperature included. Most of the earlier work was done for soda liquor which is a limiting case of kraft liquor, since only sodium hydroxide is present as a pulping agent. The soda process was used extensively to pulp hardwoods which are easier to pulp and hence require less severe pulping conditions. This is due to a lower lignin content in hardwoods. The introduction of the kraft process gave a higher pulping rate and softwoods too could then be pulped economically. Though woods have been broadly isolated into hardwood and softwood classes, each individual species has its own reaction rate (81 p614).

A first order kinetic representation is dominant and Mitchell and Yorston (76), Schwartz and Bray (84), Larocque and Maass(63), Kulkarni and Nolan (61) and Carroll (14) have derived delignification equations of the form:

$$\frac{dL}{dt} = ki*(L - Ld) \qquad 3.4.(i)$$

where ki is the kinetic constant, L the lignin present at the time t and Ld is lignin that is difficult to remove

in the last stages of the cook.

The kinetic constant, k is related to temperature by an Arrhenius type relationship and activation energy values vary from 30,000 to 35,000 cal/mole for kraft cooks. The effect of hydroxide and sulphide concentration in the liquor is included in the effective rate constant calculation as a linear relationship.

These earlier kinetic models related to only the "bulk" reaction. Kleppe (59) and Stillman (93) state that the pulping reaction occurs with three different rates, "extractive", "bulk" and the "residual", while Kleinert (55, 58) mentions only the "bulk" and "residual" rates. The "extractive" rate corresponds to the easily removable and readily accessible wood constituents, the "bulk" to describe the majority of the reaction and the "residual" for the last few percent of least accessible and most difficult amount of wood constituent to remove. These differing rates are assumed to be first order. Stillman derived a relation to identify the breakpoint between bulk and residual lignin as a function of lignin and liquor concentrations and the cooking temperature. The extractive rate is based on extrapolating the bulk reaction curve to zero cooking time

and noting the difference between the actual and bulk lignin content obtained by extrapolating the curve. Stillman plotted data from Hobden (41), Kleppe (59), and Aurell and Hartler (1, 2) to show the three rates.

Mitchell and Yorston (76), Stillman (93) and Wilder and Daleski (102) too used a first order equation of the form :

$$\frac{dL}{dt} = - k*L \qquad 3.4.(ii)$$

to describe the reaction kinetics. The rate constant k is a function of both the kraft liquor component concentrations

$$k = k_1*(OH^-) + k_2*(S^{2-})**a \qquad 3.4.(iii)$$

where (OH^-) is the effective sodium hydroxide concentration, (S^{2-}) is the sulphide concentration and 'a' is the exponential power for sulphide which varies with wood species. Daleski (21) obtained 38 Kcal/mole for k_1 and 26.9 Kcal/mole for k_2.

Stillman uses the same form of equation for pulping of seven hardwood and softwood components. The effective alkali relationship is based on data from Martin (72). Since sodium sulphide was found to have a large effect on carbohydrate removal in the initial portions of the cook, a

effective concentration for sodium sulphide is evaluated to obtain a good correlation. To calculate the three different reaction rates for bulk, extractive and residual phases, factors which multiply the Arrhenius constants are calculated.

Findley and Nolan (25) derived a model for two simultaneous reactions for wood components in neutral sulphite pulping. They are:

$$\frac{dYa}{dt} = -Ka*Ya$$

$$\frac{dYb}{dt} = -Kb*Yb \qquad 3.4.(iv)$$

$$\text{and } Y = Ya + Yb + 43$$

where Ya and Yb are wood fractions with velocity constants Ka and Kb respectively and Y is the wood yield with 43% unreacted wood. Johnsson (49) uses a somewhat similar model for his kinetics.

The latest models are from LeMcn and Teder (67) and Smith and Williams (88) and they use the following equation :

$$-\frac{dL}{dt} = K_1*L*(OH^-) + K_2*L*(OH^-)*(HS^-)**b \qquad 3.4.(v)$$

where (OH^-) is the effective alkali and (HS^-) the bisulphide concentration. The exponential constants used by Smith and

Williams are unity and they have used the same form of equation for five wood components: fast and slow reacting lignin, cellulose, xylan and mannan. Kinetic data is derived from actual laboratory cooks of hardwood and softwood species. LeMon and Teder have used the equation only for lignin and have fractional values for the exponential constants rather than unity.

3.4.3 Kinetic Model

The kinetic model in this work is based on Stillman's (93) model. Therefore the kraft liquor components, sodium hydroxide and sodium sulphide are considered as actual hydroxide and sulphide in the kinetic equation instead of effective alkali and bisulphide. The total hydroxide or alkali concentration is taken as the sodium hydroxide in the liquor plus the amount generated from the sodium sulphide hydrolysed. For the sodium sulphide, instead of assuming fifty percent hydrolysis as is defined for the effective alkali, Martin's (72) data for hydrolysis is used and the actual hydrolysis calculated. Sodium sulphide was considered as the sulphide although hydrolysis generates bisulphide or hydrogen sulphide. An

effective scdium sulphide concentration is evaluated for degradation of carbohydrates, as the sulphide is responsible for a higher pulping reaction in the earlier parts of the cook (59, 101).

The reaction kinetics are considered first order with respect to the wood components and the contribution of sodium hydroxide and sodium sulphide to the kinetic constant additive. The relevant equations follow:

$$\frac{dXn}{dt} = -Ko*Xn \qquad 3.4.(vi)$$

where Ko is the reaction constant and Xn the wood component concentration in the nth digester section. The constant Ko is equal to:

$$Ko = K_1*(OH^-) + K_2*(S^{2-})**a \qquad 3.4.(vii)$$

The exponent 'a' is 0.631 for hardwoods and 0.681 for softwoods (93). The constants K_1 and K_2 are for the hydroxide and sulphide respectively and related to the cooking temperature, T, by the Arrhenius equation and a reaction phase factor, B.

$$\text{eg. } K_1 = B_1*\exp(A_1 - E_1/T) \qquad 3.4\ (viii)$$

The constants A, B and E for various wood components are shown in Table 2.

Lignin and xylan are assumed to react with three different rates, extractive, bulk and residual while mannan is considered to have only extractive and bulk rates. The extractive amount is calculated by extrapolating the bulk reaction curve to zero cook time and the difference between the component concentration thus obtained is the actual value assumed to be in the fast extractive phase. The breakpoint between the bulk and the residual phases is calculated from the wood compositions and the cooking conditions, liquor concentrations and the temperature (93).

3.4.4 Reasons for Kinetic Model

The reaction model described above was chosen because it seems to match the physical realities of the cooking process. The complex sulphur ion hydrolysis was not used as it is difficult to determine the exact quantities involved. A fifty percent sulphide hydrolysis concept of effective alkali was not used for similar reasons, instead sulphide hydrolysis is calculated and the alkali concentration evaluated in terms of measurable liquor components. The differing rates of reaction observed for some wood components are included as cooking does sometimes go into the residual reaction phase, although this is not desirable as the yield loss at this stage is greater than the benefit gained by the extra lignin removal. This has been observed and reported by several authors, as mentioned earlier (1, 21, 58).

Table 2 Kinetic Rate Constants for Softwood and Hardwood Species

Rate Constant, k = B*exp(A - (E/Temperature))

where A & E are the Arhennius constants and B is a reaction phase factor which has a value greater than one for the extractive phase, unity for the bulk phase and less than one for the extractive phase. Wood components and their rate phase factor, if used are shown in the table.

WOOD COMPONENT	HYDROXIDE A	HYDROXIDE E	HYDROXIDE B	SULPHIDE A	SULPHIDE E	SULPHIDE B
			SOFTWOOD			
Lignin	30.223	31043.0	20.3 Extractive 0.2519 Residual	33.531	26012.0	5.46 Extractive 0.2519 Residual
Cellulose	31.356	27553.0	1.0	32.321	27553.0	1.0
Mannan	31.916	26737.0	256.7 Extractive	32.988	26737.0	256.7 Extractive
Xylan	33.125	26737.0	5.48 Extractive 0.1282 Residual	34.246	26737.0	5.48 Extractive 0.1282 Residual

... continued

Table 2 (continued)

WOOD COMPONENT	HYDROXIDE A	HYDROXIDE E	HYDROXIDE B	SULPHIDE A	SULPHIDE E	SULPHIDE B
		HARDWOOD				
Lignin	40.626	32175.0	23.8 Extractive 0.2137 Residual	32.074	24471.0	6.40 Extractive 0.2257 Residual
Cellulose	32.085	27553.0	1.0	33.050	27553.0	1.0
Mannan	31.916	26737.0	256.7 Extractive	32.988	26737.0	256.7 Extractive
Xylan	32.432	26737.0	21.90 Extractive 0.0641 Residual	33.553	26737.0	21.90 Extractive 0.0641 Residual

CHAPTER FOUR

DESCRIPTION OF MODEL

The Kamyr continuous digester model derived in this work could, based on mathematical modelling principles, have been anywhere between two extremes. A set of trivial linear algebraic equations could have been derived for the digester variables using input-output plant data. This may have accomplished the job but only within a certain limited operating range and thus have severe restrictions. A rigorous model expressed in terms of several nonlinear partial differertial equations, would have been mainly a mathematical and computing exercise and would have served little purpose in what this project was eventually aimed at, i.e. control of the cooking process. An intermediate approach was taken instead and this helped in making the mathematical and computational requirements of the model reasonable but without compromising the physical realities of the system.

In this chapter the derivation, solution technique, computer programming and testing of the digester model are

presented.

4.1 Derivation of Model Equations

Since the continuous Kamyr digester is a distributed parameter system, a partial differential equation was derived for a general wood component concentration. The equation is presented in Appendix A.1. This equation was reduced to an ordinary differential equation which applies to each of the N sections that the digester is divided up into. This makes each section a 'lumped parameter' or 'stirred tank' system. The remaining equations are derived directly for such a system. The alternate approach would have been to directly start from the concept of equivalence of a tubular reactor to a series of stirred tanks and to develop the model equations from there onwards. This was not done as the existing mathematical derivation makes the set of boundary conditions for the discretized case more obvious.

Material and energy balances for thirteen state variables were derived for an ideal stirred tank, giving a set of thirteen coupled, first order, nonlinear ordinary

differential equations. This set of equations is shown in Table 3 and again in Appendix A.2.

The partial differential equation (Eqn A.1.1) was simplified by neglecting the radial and angular components and discretizing along the vertical axis. Diffusion of the solid phase wood components is assumed negligible, which eliminates the second order terms, leaving convection, total reaction and unsteady state terms. Discretization of the initial conditions led to an initial entering condition at the top of the digester and an initial profile of starting values for each of the N digester sections.

The first equation in the set of equations is for the wood density in a digester section and this is essentially to calculate the wood flow rate leaving the section. The flow rate into the first section depends on the chipmeter speed and the blow flow out of the digester. The flow out of a digester section depends on the entering flow and the wood density in that section. The wood density is related to the degree of compaction which is a measure of the reduction in wood volume per unit mass. The compaction relationship is a dynamic one and is based on the amount of cooking that the chips have been subjected to in the

digester, i.e. their H-factor. The next four equations are the wood component balances for lignin, cellulose, mannan and xylan. These equations include flow by convection and their depletion by first order kinetics that were shown in the last chapter. Liquor component balances in the free and entrapped liquors are for the hydroxide, sulphide, and reaction products and include convection flow and mass transfer of the components between the entrapped and free liquor volumes in the section. The depletion of cooking chemicals is calculated from the rate of reaction of wood constituents and their corresponding stoichiometric coefficients and is deducted from the entrapped liquor. The mass balance for the reaction products or dissolved solids in the entrapped and free liquors contain terms similar to the chemical balances. The rate of generation of these dissolved solids is equal to the rate of depletion of wood and cooking chemicals.

The energy balances are evaluated for the wood plus entrapped liquor, and the free liquor. Here modifications are made in the free liquor calculations to account for external heater and extraction flows. Perfect mixing of the external stream and the free liquor is assumed. Terms for

Table 3 Nonlinear Digester Model Equations[1]

i) Calculation of Reaction Rate Terms for Wood Components

Lignin-Hydroxide Rate = K1*Wood Mass*(Lignin(n+1)*0.01)*Total Hydroxide
Lignin-Sulphide Rate = K2*Wood Mass*(Lignin(n+1)*0.01)*Sulphide**ENA2S

Cellulose-Hydroxide Rate = K3*Wood Mass*(Cellulose(n+1)*0.01)*Total Hydroxide
Cellulose-Sulphide Rate = K4*Wood Mass*(Cellulose(n+1)*0.01)*Sulphide for Carbohydrates

Mannan-Hydroxide Rate = K5*Wood Mass*(Mannan(n+1)*0.01)*Total Hydroxide
Mannan-Sulphide Rate = K6*Wood Mass*(Mannan(n+1)*0.01)*Sulphide for Carbohydrates

Xylan-Hydroxide Rate = K7*Wood Mass*(Xylan(n+1)*0.01)*Total Hydroxide
Xylan-Sulphide Rate = K8*Wood Mass*(Xylan(n+1)*0.01)*Sulphide for Carbohydrates

where Total Hydroxide is the Entrapped Liquor Hydroxide and the Hydroxide from Sulphide Hydrolysis, and ENA2S is the exponent for the Lignin-Sulphide equation

ii) Calculate Sulphide Depletion

Sulphide Depletion = 0.092857*Lignin-Sulphide Rate

iii) Calculate Hydroxide Depletion, the first equation is evaluated only in the Impregnation Zone and the calculation is Zero otherwise

Hydroxide Depletion = 0.114595*Extractive Rate + 0.210526*Uronic Acid Rate + 0.140233*Acetyl Rate

Hydroxide Depletion = Hydroxide Depletion + 0.104712*Lignin-Hydroxide Rate + 0.454545*(Total Xylan Rate) + 0.370370*(Total Mannan and Cellulose Rates)

[1] These thirteen equations constitute the model used in each digester section (see also Appendix A)

... continued

Table 3 (continued)

iv) Calculate Wood Depletion and Solid Generation Rates

Total Wood Depletion Rate = Sum Total of All Wood Component Rates

Total Solid Generation Rate = Total Wood + Total Chemical Depletion Rates

v) Wood Flow Rate Equation, Equation Number 1

d(Wood Flow(n+1))/dt = Wood Density Function*Volumetric Wood Rate(n+1)

vi) Wood Component Mass Balances, Equation Numbers 2-5

d(Lignin(n+1))/dt = (Wood Flow(n)*Lignin(n) - Wood Flow(n+1)*Lignin(n+1)
- (Total Lignin Rate*100.0))/Wood Mass

d(Cellulose(n+1))/dt = (Wood Flow(n)*Cellulose(n) - Wood Flow(n+1)*Cellulose(n+1)
- (Total Cellulose Rate*100.0))/Wood Mass

d(Mannan(n+1))/dt = (Wood Flow(n)*Mannan(n) - Wood Flow(n+1)*Mannan(n+1)
- (Total Mannan Rate*100.0))/Wood Mass

d(Xylan(n+1))/dt = (Wood Flow(n)*Xylan(n) - Wood Flow(n+1)*Xylan(n+1)
- (Total Xylan Rate*100.0))/Wood Mass

vii) Mass Transfer Rates

Hydroxide Mass Transfer = Mass Transfer Coefficient*Area*(Free Liquor Hydroxide(n+1)
- Entrapped Liquor Hydroxide(n+1))

Sulphide Mass Transfer = Mass Transfer Coefficient*Area*(Free Liquor Sulphide(n+1)
- Entrapped Liquor Sulphide(n+1))

Solids Mass Transfer = Mass Transfer Coefficient*Area*(Free Liquor Solids(n+1)
- Entrapped Liquor Hydroxide(n+1))

... continued

Table 3 (continued)

viii) Entrapped Liquor Mass Balances. Equation Numbers 6-8

d(Entrapped Liquor Hydroxide(n+1))/dt = (Vol Flow In*Entrapped Liquor Hydroxide(n)
- Vol Flow Out*Entrapped Liquor Hydroxide(n+1)
+ Hydroxide Transfer - Hydroxide Depletion)/EL Volume

d(Entrapped Liquor Sulphide(n+1))/dt = (Vol Flow In*Entrapped Liquor Sulphide(n)
- Vol Flow Out*Entrapped Liquor Sulphide(n+1)
+ Sulphide Transfer - Sulphide Depletion)/EL Volume

d(Entrapped Liquor Solids(n+1))/dt = (Vol Flow In*Entrapped Liquor Solids(n)
- Vol Flow Out*Entrapped Liquor Solids(n+1)
+ Solids Transfer + Solids Generation)/EL Volume

ix) Free Liquor Mass Balances. Equation Numbers 9-11

d(Free Liquor Hydroxide(n+1))/dt = (Vol Flow In*Free Liquor Hydroxide(n)
- Vol Flow Out*Free Liquor Hydroxide(n+1)
- Hydroxide Transfer)/FL Volume

d(Free Liquor Sulphide(n+1))/dt = (Vol Flow In*Free Liquor Sulphide(n)
- Vol Flow Out*Free Liquor Sulphide(n+1)
- Sulphide Transfer)/FL Volume

d(Free Liquor Solids(n+1))/dt = (Vol Flow In*Free Liquor Solids(n)
- Vol Flow Out*Free Liquor Solids(n+1)
- Solids Transfer)/FL Volume

... continued

Table 3 (continued)

x) Heat Transfer Calculations

Heat Exchange = Heat Transfer Coefficient*Area*(Wood Temperature(n+1)
- Free Liquor Temperature(n+1)) + (Heat Transfer From Walls)

Reaction Heat Transfer = Total Wood Reaction Rate*Heat of Reaction

xi) Energy Balances. Equation Numbers 12-13

d(Wood Temperature(n+1))/dt = Wood & EL Mass Flow In*Specific Heat*Wood Temperature(n)
- Wood & EL Mass Flow Out*Specific Heat*Wood Temperature(n+1)
+ Reaction Heat Transfer + Heat Exchange)
/(Wood & EL Total Mass*Avg Wood & Liquor Specific Heat)

d(Free Liquor Temperature(n+1))/dt = (FL MassFlow In*Liquor Specfic Heat*FL Temperature(n)
- FL Mass Flow Out*Liquor Specific Heat*FL Temperature(n+1)
- Heat Exchange)/(FL Total Mass*Liquor Specific Heat)

where K1, K2,....., K8 are the Wood Component Reaction Rate Constants which are dependent on temperature. The rate constants and all the other constants, e.g. Specific Heats, Transfer Coefficients etc., are passed on from other subroutines in the program.

The notation 'n' is used for the previous section and 'n+1' for the current one when refering to the State Variables.

convective transfer between the wood and free liquor phases are included. The heat of reaction generated and the heat transfer from the walls are divided proportionately among the two equations.

4.2 Equation Solution Technique

The digester model was programmed in FORTRAN and run on an Amdahl 470 V/6 computer. Simplified flow diagrams of the program are shown in Figure 4.1, and in Appendix C.1. Detailed flow diagrams and program listings are included in a separate programmer's manual. Starting values for an initial profile are read in, estimated based on the entering and operating conditions or calculated as a steady state profile. The first half of the program for cocurrent chip and liquor flow in the impregnation, heating and cooking zones of the digester is an initial value problem. The second, or lower part of the digester which includes the quench, extraction, wash and cold blow zones have a wash flow countercurrent to the chip flow. This problem can be treated as an initial value problem also, as long as the starting values and the profile are known. The steady state

profile for the countercurrent zones has to be solved iteratively as a boundary value problem.

The initial value problem was integrated using an explicit fourth order Runge-Kutta technique (Runge-Kutta Merson) with truncation error estimation and integration step size control. The subroutine used is DASCRU, from the IMSL (International Mathematical and Statistical Library, (45)) subroutine package and was found to be the best available. A comparison of computing times and accuracy for other solution methods is given in Appendix B.1.

The steady state digester profile which is the solution of a set of nonlinear simultaneous algebraic equations is calculated using a modified form of the Newton-Raphson method. This method is called Brown's method and is available in the IMSL package as the subroutine, ZSYSTM (45). For the cocurrent problem a set of thirteen equations are solved simultaneously to obtain the steady state values of the digester variables in one section, but in the washing zone, equations for all the sections have to be setup and solved simultaneously.

4.3 Description of Computer Program

The computer program for the Kamyr digester model solves the set of nonlinear ordinary differential equations shown in Table 3 for each section of the digester. The overall program is a dynamic one and allows for cooking in the wash zone.

The program starts with real time being initialized and all the relevant flags set. The user defined flags direct the logical flow of the program according to the options specified. For example, flags can be set to specify omission of heat balances (which reduces the number of equations to be solved), plotting of profiles, which variables are to be plotted and chip history. Input data that is read in the mainline program includes physical constants, initial digester entering conditions, digester configuration data and an initial digester profile, if it is known. The zone and section volumes, internal piping and digester wall areas are all calculated for the specified digester configuration. These areas and section volumes are printed out along with the section numbers which have

screens for liquor extraction in them. A sample printout is shown in Appendix C.2. The initial digester profile is calculated next, if it has not been specified as a part of the input data.

The main processing loop starts next with two objectives: to calculate a digester profile at a certain time and to keep track of each entering wood mass so as to trace its cooking history through the digester.

The integration step size is specified and the input conditions to a section, at time t, are set to the digester entering conditions in the first section or the initial condition of the previous section at the same time. The outlet conditions from the section are set to the initial conditions of the section at time t. The set of equations are then solved as an initial value problem and conditions at time $t + \Delta t$ calculated. The section temperatures are estimated by assuming them to be equal to the ones in the last time interval. Next, a check is made whether the section has a screen and/or an external entering flow such as one of the heater streams, and if so, a perfect mixing calculation is made for the chemical concentrations and temperature of the entering free liquor stream to the

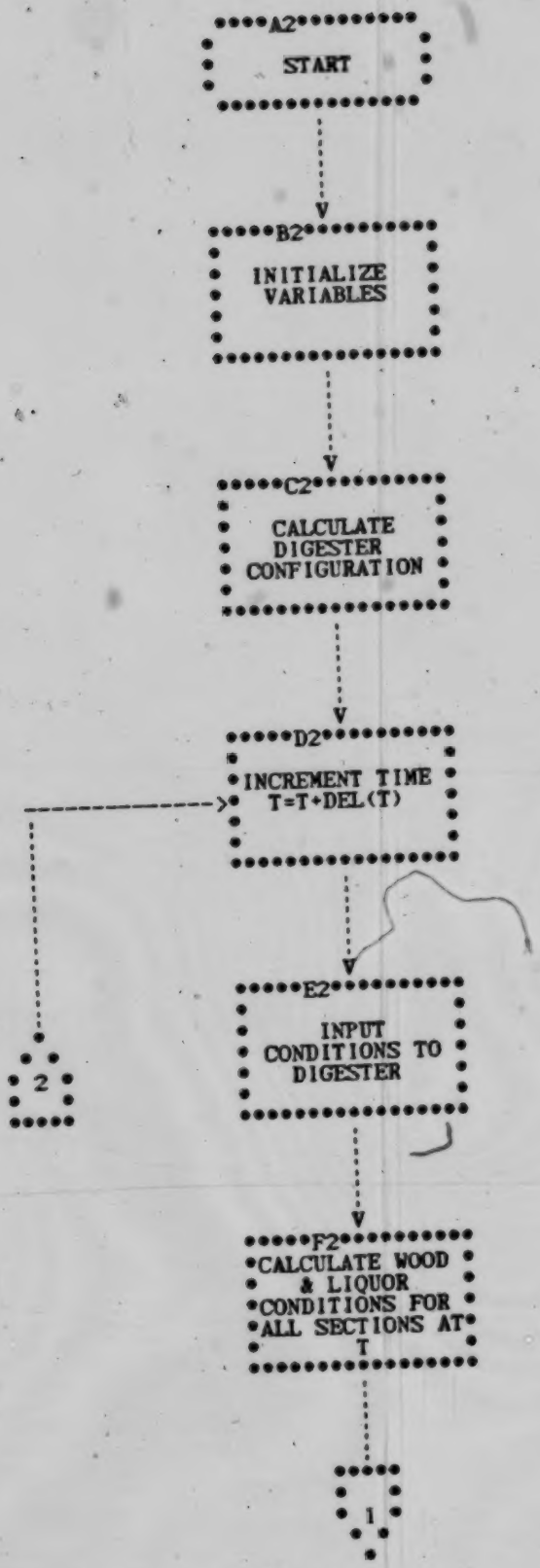


Figure 4.1 : Simplified Program Flow Diagram

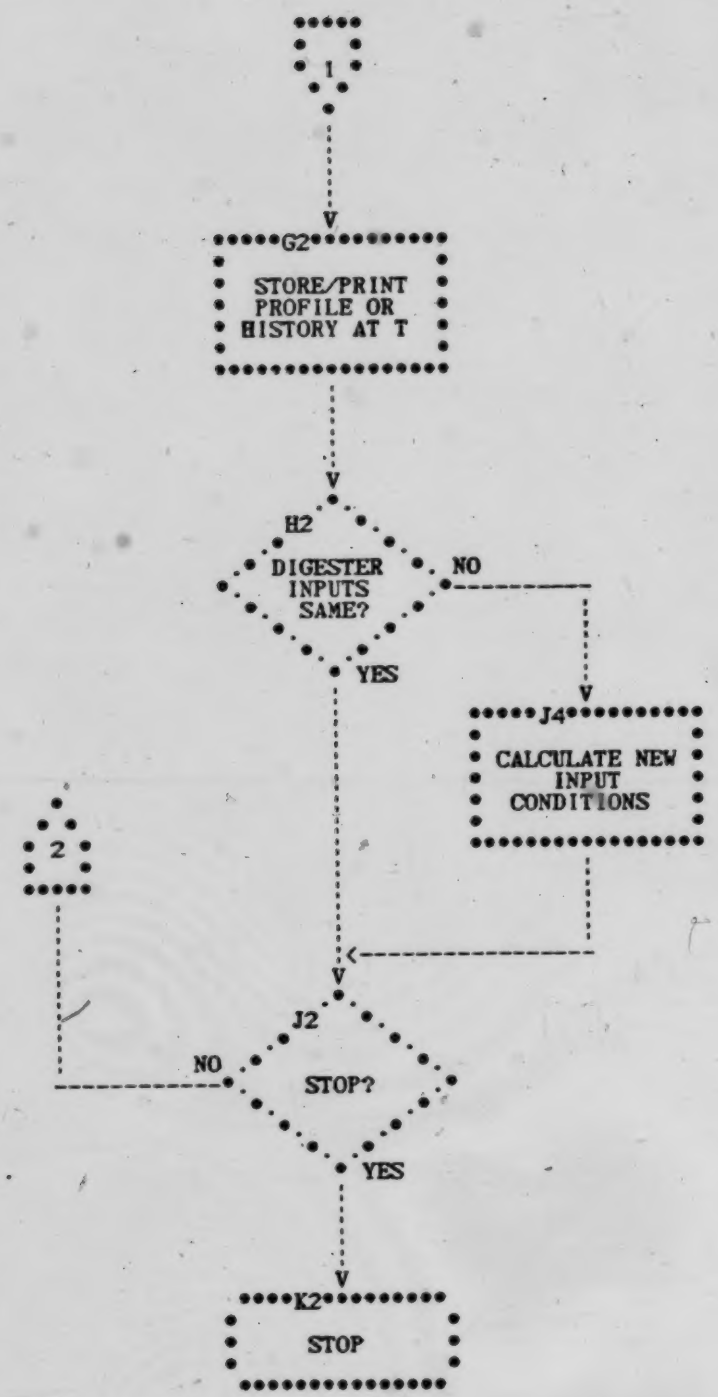


Figure 4.1 continued.. Simplified Program Flow Diagram

section. The rate constants, mass transfer coefficients, compaction in the section, wood mass and free and entrapped liquor volumes are calculated and the thirteen first order differential equations set up. The equations are solved by a Runge Kutta type routine from the IMSL subroutine package. If the section temperature calculated from the energy balance is within a specified limit of the assumed value, then the wood conditions are updated. Otherwise the section temperatures are iterated upon after recalculating the temperature dependent variables. For the countercurrent flow sections, the starting values are estimated first and only the steady state problem is solved differently. The dynamic boundary value problem is converted to an initial value problem using the known countercurrent stream entering conditions or the calculated 'steady state' profile which has been solved as a boundary value problem.

After calculations are made for all digester sections, the profile is printed out and before calculations are repeated from the top, the current entering or process operating conditions are checked. If they are different, a new set of conditions are calculated.

At this stage further calculations and execution

are stopped if one of the stopping criteria are met which are time, number of profiles or when the character string 'STOP' is read in.

4.4 Testing of Model

The model was tested in three parts. First, the working of individual subroutines, next numerical comparison of integration methods and last the testing of the overall program.

The program subroutines were individually tested against published data and found accurate for modelling purposes within the digester operating range. Routines tested first were those that could be checked with a hand calculator. Such routines were the ones for the digester configuration, residence time, digester entering conditions and external flow calculations. The water density calculation routine which is used to evaluate liquor density change versus temperature was checked in a temperature range of 25 to 200 °C. The results were as expected since a second order polynomial was fitted using data values in the same range. The cooking liquor contains sodium sulphide that hydrolyses to sodium hydroxide. The results from the

hydrolysis routine were compared with data from Martin (72). These results were reasonable at most points but had a maximum error of 12%. The largest errors were at temperatures around 25 °C and at high temperatures and sulphidities which are out of the usual operating range.

The integration problem for the differential equations was such that a very efficient routine was required. Fourth order Runge Kutta and Predictor Corrector methods were examined. These routines were taken from the IMSL (45), IBM Scientific Subroutine Package (83) and some were written as a part of the whole digester modelling package. Computer run times and accuracy using the IMSL routine were not as good as with the fourth order Runge Kutta routine, when tested against simple linear and stiff systems. The Runge Kutta routine was not able to handle the severe nonlinearities when solving the system of equations in the proximity of the digester heating zones. This was apparently due to a constant integration step size that could not be reduced in such cases. The IMSL routine which has integration step size control was then chosen due to this reason.

The steady state solution problem was solved using

the Brown's modified Newton-Raphson method (IMSL (39)). This IMSL routine was also found to be superior as it is at least quadratically convergent and the number of functional evaluations per iterative step are of the order of 0.5*(N*N + 3*N) as opposed to N*N for the Newton Raphson method.

The kinetic model testing was done by writing a model for a batch digester. This model was basically the same as for the continuous case since the same number of differential equations were to be solved. The only difference was the absence of flow terms and adjustments had to be made accordingly. The integration time was the actual cooking time. For testing purposes actual laboratory cook data was used and so the heat balance equations could be neglected as in most of the cases the data was collected under isothermal conditions or the temperature profile was explicitly known. Data from Daleski (21) and from Smith and William (88) was used. The kinetic parameters used for the first set of runs were supplied by Consolidated-Bathurst Ltd. (6), but these values had to be tuned to get better results. Some of the batch cook runs are shown in Appendix B.3. It was the constants obtained from these runs that were used for subsequent simulations. These constants are

shown in Table 2.

Trivial testing of the program was to check the overall working of the program. Since individual routines, the integration method, and the kinetic model were already tested, it was assumed that any other irregularities in the model would become apparent in this testing. The trivial testing included such cases as where the reaction rate constants were set to zero and the digester started up from a constant set of initial conditions. The results from this case were that the digester wood profile remained constant throughout. A similar test was starting with a digester of fully cooked chips and then setting the reaction constants to zero. This run showed the movement of the cooked chips down the digester and the top steadily filling up with the uncooked chips. The dynamics of the model were tested by a similar start up but with the regular kinetic constants in use. The dynamics of the model were also tested by allowing the digester to reach a steady state value and this value compared with that from the steady state model. The results were fairly close and, since the same results were obtained from two independent programs, was a check on the dynamic program. Since actual digester operating data was lacking a

direct check could not be made. However it was expected that the model would be able to come close to the actual Kappa number if data were available especially since cooking in the wash zone was included.

CHAPTER FIVE

OPEN LOOP DIGESTER SIMULATION RESULTS

Several open loop simulation runs were conducted using different values for operating variables, such as alkalinity and cooking temperature, to show their effect on internal conditions in the digester as well as on the end product. Most figures, e.g. Figure 5.2, are plots of the state variable of interest versus digester height. Digester height is plotted as the vertical axis so that there is a direct correspondence between vertical position on the figure and vertical position in the actual digester. For all the runs presented in this chapter, the digester was modelled by a total of 24 sections and hence the results produced by the model consist of 24 values of each variable, at each time step. For a given profile, the 24 points were fit by spline functions and plotted as a continuous curve so that the dynamic changes in the profiles could be followed more easily. Figures 5.9 and 5.10 are referred to as 'history plots' since they show the actual state of a pulp

sample from the time it entered the top of the digester until it exited via the blow line. After extended periods of steady state operation the history plots become equal to the instantaneous profiles. However, during transient periods these plots show the history of the current exit pulp and hence would be of assistance to the operators of downstream process units. The digester physical parameters and operating conditions for run #1 are presented in full in Appendix C.2.

The simulation runs are grouped into six sets and are discussed in the following sections. The sets are :

i) A run from constant initial conditions, as in the startup of a digester, to a steady state,
ii) alkaline concentration changes,
iii) heater or cooking temperature changes,
iv) variation of cook zone residence time, by altering the production rate and by varying the length of the cook zone, through changing quench and extraction conditions,
v) production and grade changes
and vi) a species change.

Each set of runs is discussed separately and the overall results from these runs are summarized in the last section.

5.1 Digester Run from Constant Initial Conditions to Steady State

This run illustrates the ability of the model to simulate large dynamic changes. The digester was assumed to have constant initial profiles of fresh uncooked chips and the initial entrapped and free liquor concentrations throughout the digester were set to those entering at the top of the digester. The entrapped and free liquor temperatures in the different zones were equated to the temperatures of the external flows entering the respective zones. A sample printout of the initial profile is shown in Appendix C.2. The digester reaches a steady state after about ten hours whereas the total residence time was approximately six and a half hours. This final steady state is the 'base case' with which other runs are compared and is

used as the starting initial profile for the subsequent perturbation examples.

In Figure 5.1, the wood yield profiles are drawn. The first profile at time zero is constant at one hundred percent, since no wood is assumed to have reacted at the start. The first or impregnation zone was at a temperature of 90 C and the entrapped liquor concentrations are small hence there is little reaction in this zone and the steady state is reached in less than an hour. Most of the yield loss at this stage is for the easily removable wood components such as acetyls, etc. The heater and cook zones have the temperature of the upper and lower heater streams and the wood reacts rapidly as most of the extractive phase wood components are removed within the first five minutes. In the extraction zone the cooking temperature is reduced and the spent liquor removed, which cuts off the reaction substantially and this is clearly apparent from the first few profiles. As cooking is allowed to proceed into the wash zone, the reaction causes the wood yield to decrease but not as much as in the cooking zones since the temperatures and chemical concentrations are lower. The profiles at later times show a lower yield than before which

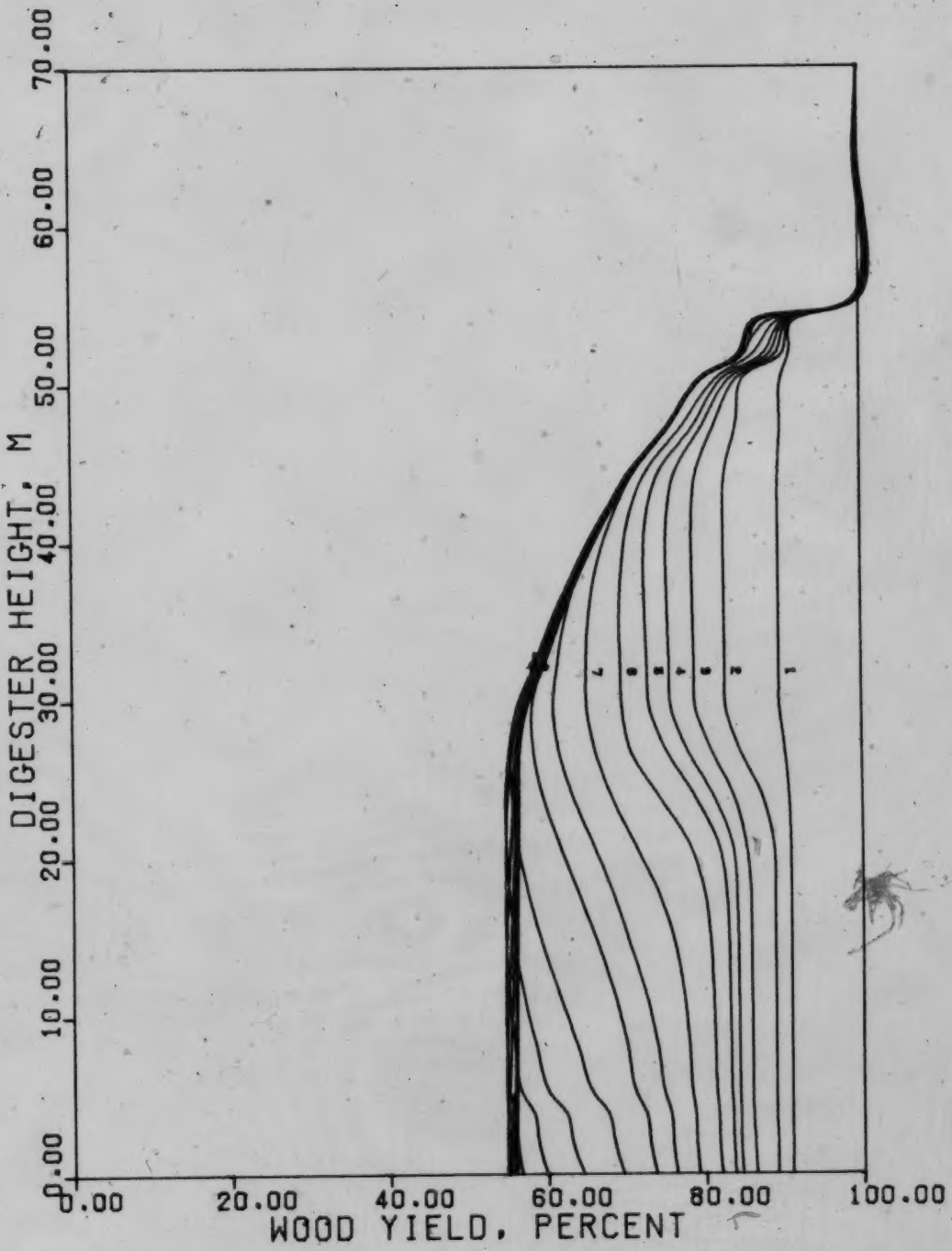


Figure 5.1 : Wood Yield Profiles for Run #1 showing 25 profiles from Startup to Final Steady State (The profiles are at 1, 5, 10, 15, 20, 30, 50, 75, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550, 600, 650, 700, 750, 800, 850 and 900 minutes respectively)

is due to the movement of cooked chips from the upper zones.

The wood component profiles for lignin, mannan and xylan, Figures 5.2 - 5.4 respectively, follow the same general pattern as the yield profiles. The initial concentration of 100% was 26.6 kg/100 kg ODW (Oven Dry Wood) for lignin, 16.2 kg/100 kg ODW for mannan and 9.5 kg/100 kg ODW for xylan. The residual percentage is higher for mannan and xylan due to their lower reaction rates. The mannan extractive amount is about 55% and is larger than the rest so most of the mannan reacts by the time the chips pass the heating zones. The xylan extractive content and rate is lower and comparatively less of it reacts in the same period. The final Kappa number at steady state was 26.2 and the yield 56 percent. These results are within the range of typical industrial operations.

The entrapped and free liquor hydroxide profiles are plotted in Figures 5.5 and 5.6 respectively. The sulphide plots are omitted since the alkalinity is directly related to both and and the sulphide curves would be similar. The entrapped liquor concentration is 15% of the free liquor concentration at the top of the digester. Further down the digester the concentration difference

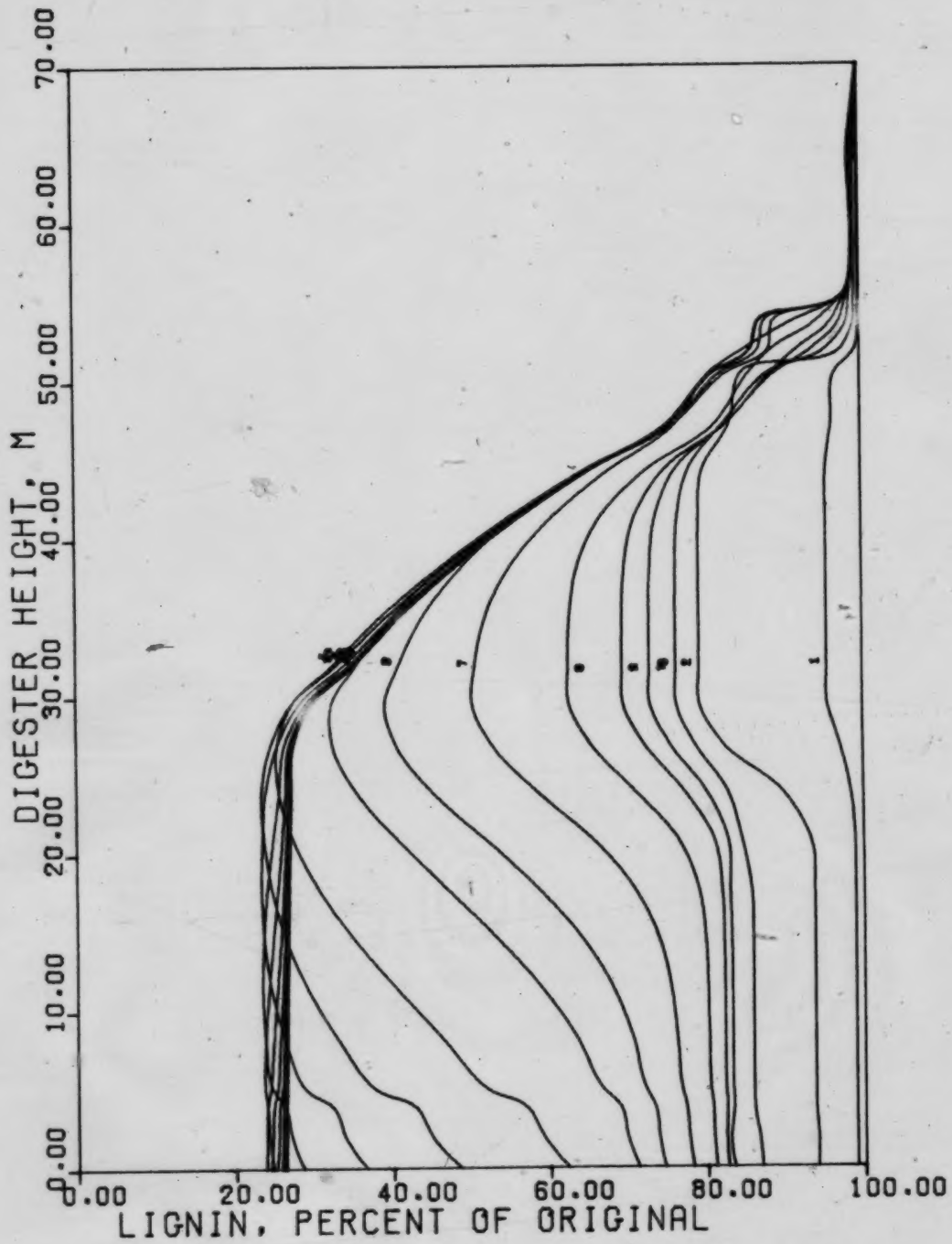


Figure 5.2 : Lignin Profiles for Run #1
(Initial Lignin Concentration 26.6 kg/100 kg ODW)

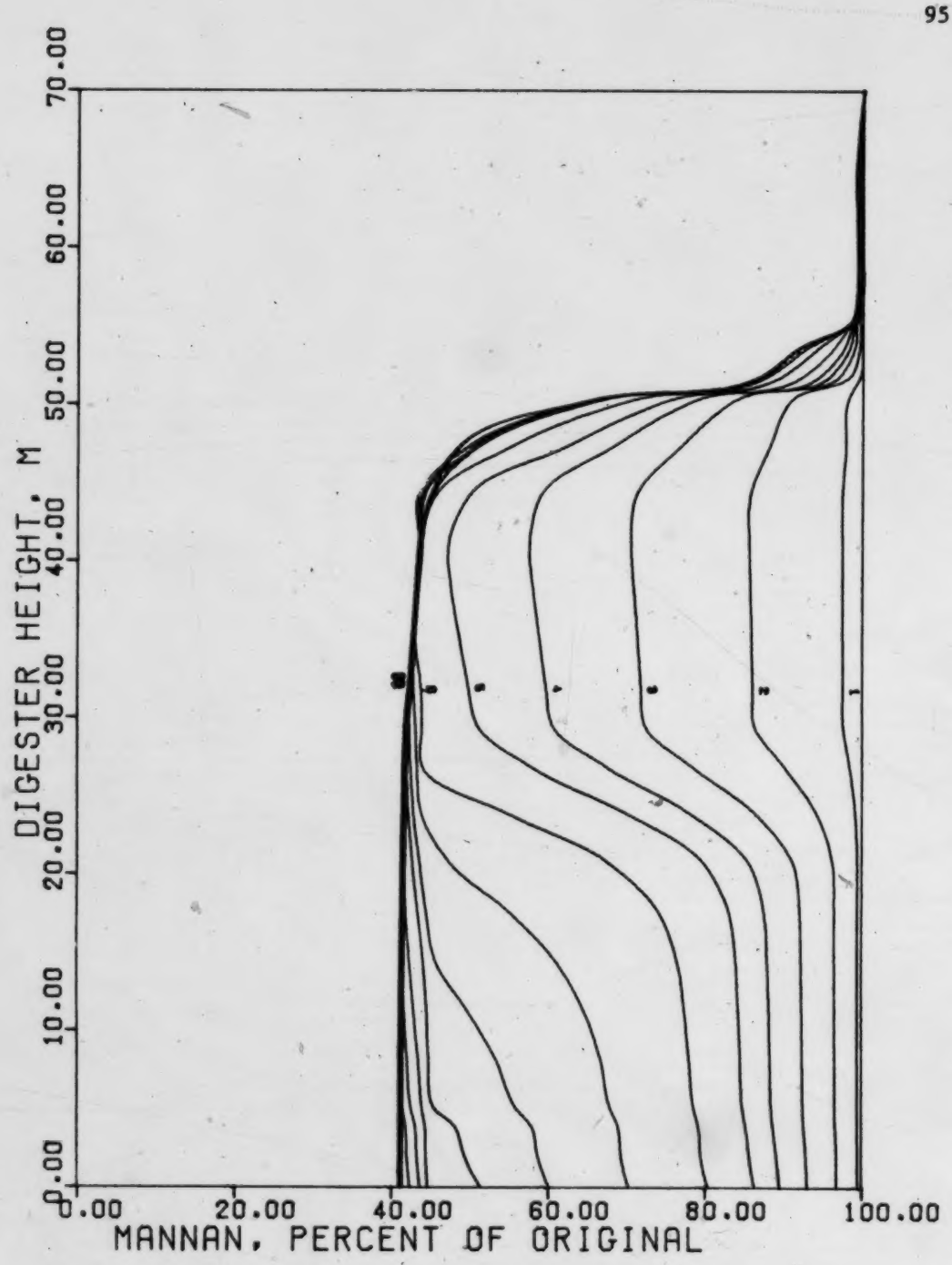


Figure 5.3 : Mannan Profiles for Run #1
(Initial Mannan Concentration 16.2 kg/100 kg ODW)

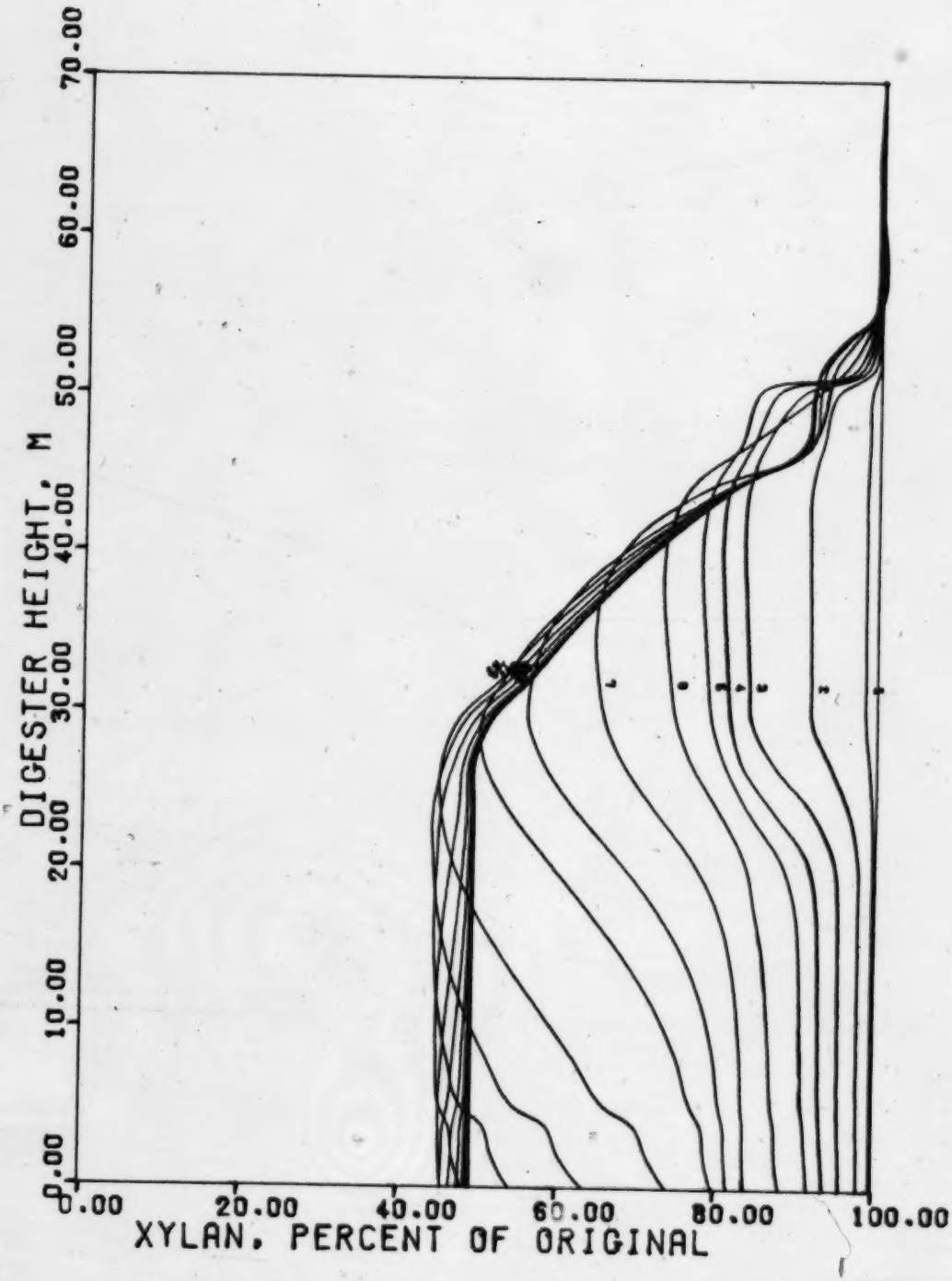


Figure 5.4 : Xylan Profiles for Run #1
(Initial Xylan Concentration 9.5 kg/100 kg ODW)

between the two phases gets smaller and the mass transfer rate decreases. The entrapped concentration attains a maximum value after one hour and then decreases until a steady state value is reached. To clearly demonstrate the transients that are involved, the profiles are split up and the ones from the initial to the maximum are plotted on the left half of Figure 5.5 and the rest on the right. The free liquor profiles on the contrary have the maximum value at the start and the concentration profiles show a decrease until a steady state is reached. The two sets of liquor concentration profiles demonstrate the combined effect of reaction, chemical usage, diffusion mass transfer in the chip and washing, along different points on the curves.

Since in the early stages of the cook, diffusion is the controlling factor rather than reaction rate, the entrapped liquor concentration reaches a maximum value at about sixty minutes whereas the free liquor concentration falls to half its original value in the same time. The reaction rate from here onwards is controlling and the entrapped liquor concentration eventually decreases to a steady state. The steady state entrapped liquor curve demonstrates the predominance of diffusion in the

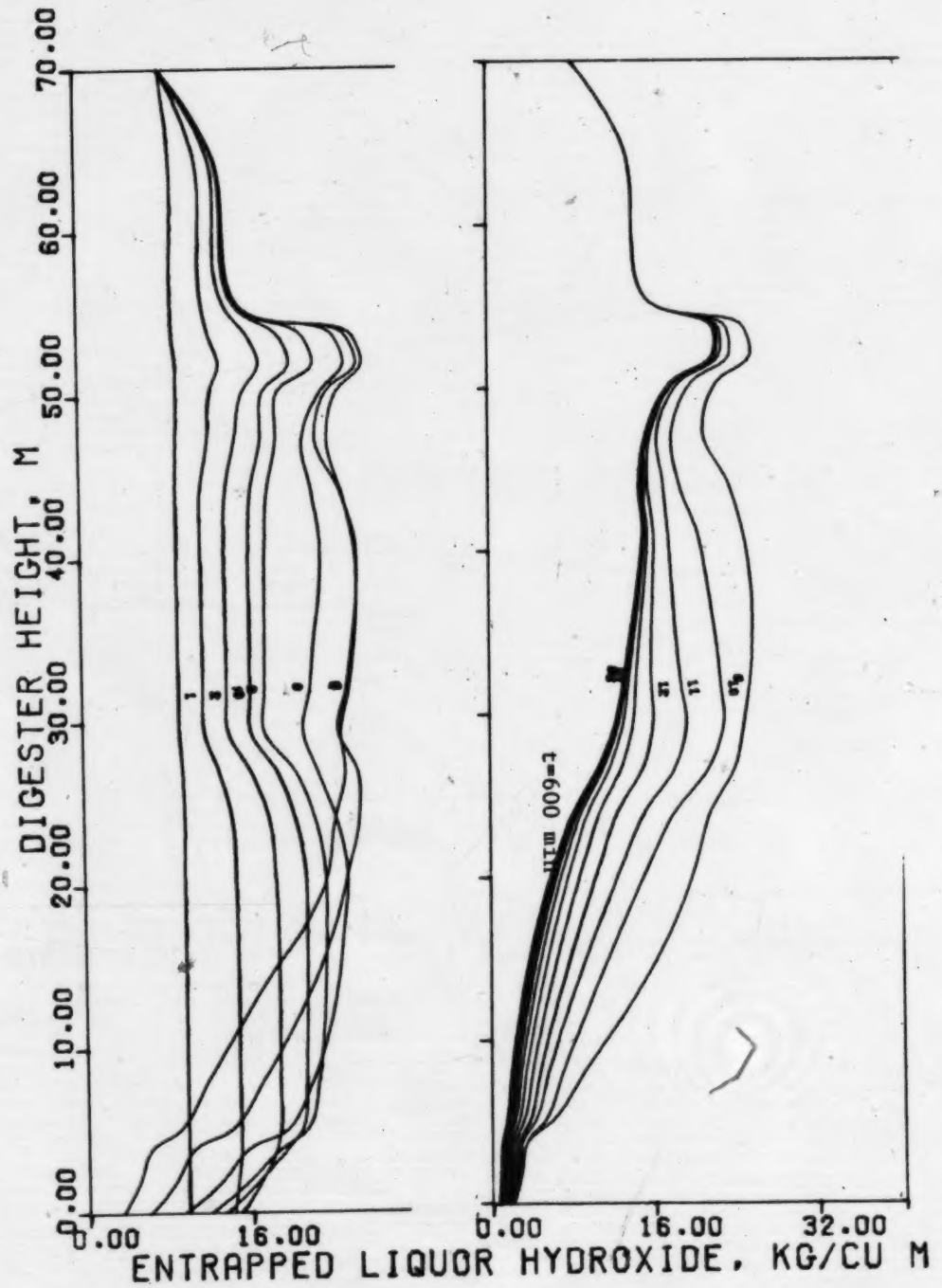


Figure 5.5 : Entrapped Liquor Hydroxide Profiles for Run #1

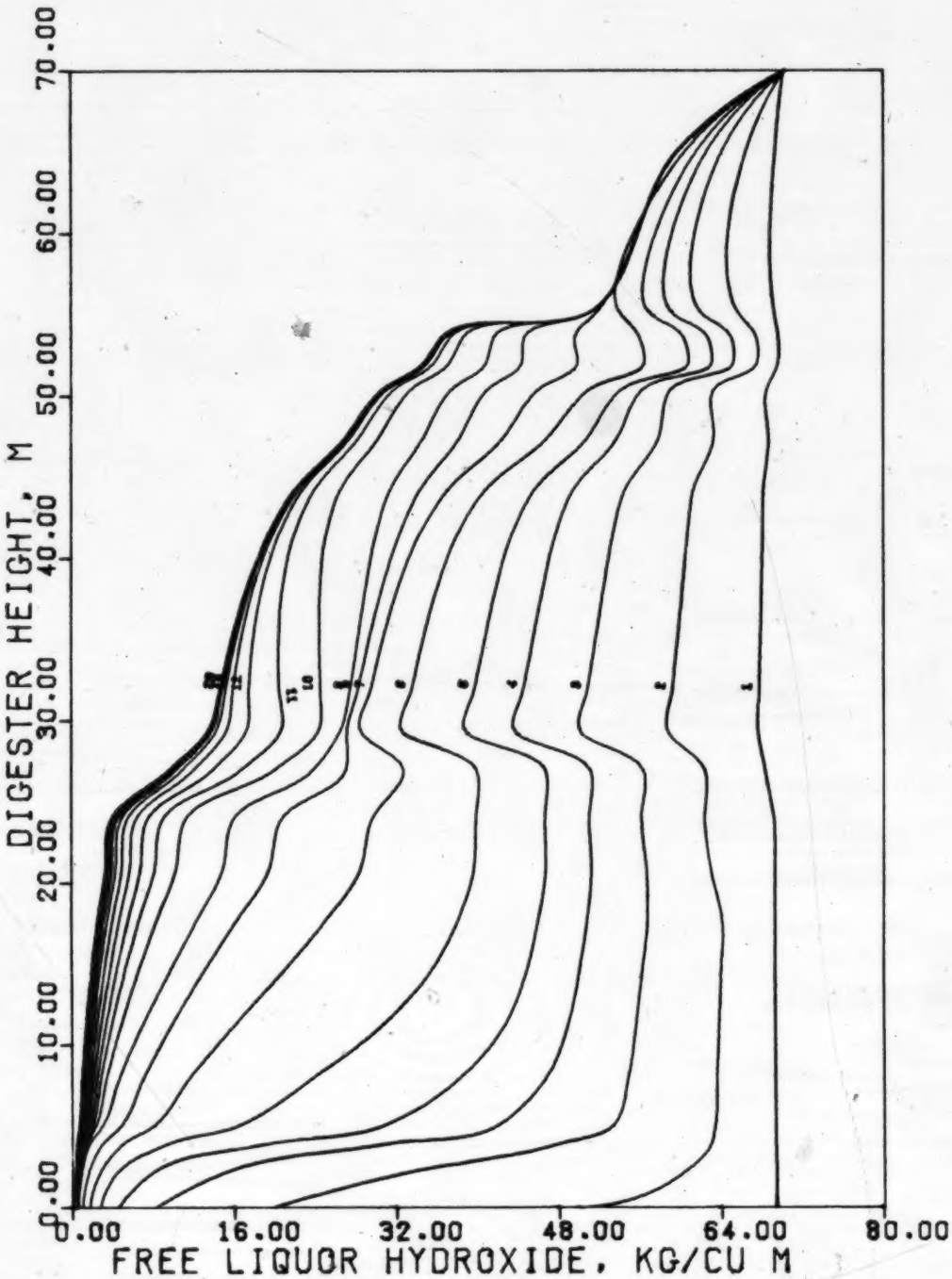


Figure 5.6 : Free Liquor Hydroxide Profiles for Run #1

impregnation zone as the concentration reaches a maximum value close to the upper heater zone. The concentration below the upper heater zone falls steadily as reaction becomes the controlling factor. At the quench/extraction screens, there is a further drop due to mixing of the cocurrent spent and quench liquor and the countercurrent wash flow. A clean water wash is used and the entrapped chemical reduces substantially due to washing, before the chips leave the digester.

The free liquor hydroxide profiles decrease throughout the digester as the chemicals diffuse into the entrapped liquor. The rate of transfer is dependent on the concentration differential and hence the reaction rate. The impregnation zone has little reaction consequently there is only a slight decrease until the upper heater zone where there is a sudden decrease. The concentration decreases further in the cook zone. The higher values in the wash zone at earlier times are due to the initial concentration profile in the zone. The movement of countercurrent wash liquor from the bottom which displaces some of the free liquor is more apparent in the earlier profiles.

The total dissolved solids or reaction products in

the entrapped liquor are shown in Figure 5.7. These curves move in the opposite direction to the chemical reactant curves and a maximum value is reached at the quench/extraction zones. This value decreases further down the digester as reaction products are washed out from the chips. The effect of the wash heater near the digester exit is noticable in the curves with a small bend at that point. This is due to a higher mass transfer coefficient which causes an improvement in the washing efficiency.

The wood chip and entrapped liquor temperature, upon which the reaction rate is dependent, is plotted in Figure 5.8. The temperature reaches steady state first in the impregnation zone since there is limited reaction and no external heating flows and the zone temperature is dependent solely on the entering chip and liquor temperatures. On leaving the impregnation zone the chips rapidly attain the temperature of the upper and lower heater streams. Then as the chips pass through the cook zone their temperature rises by another six degrees from the exothermic heat of reaction. The quench flow produces a rapid drop in this temperature but this is still higher than the temperature in the wash zone. The temperature effect of the cold blow and the wash

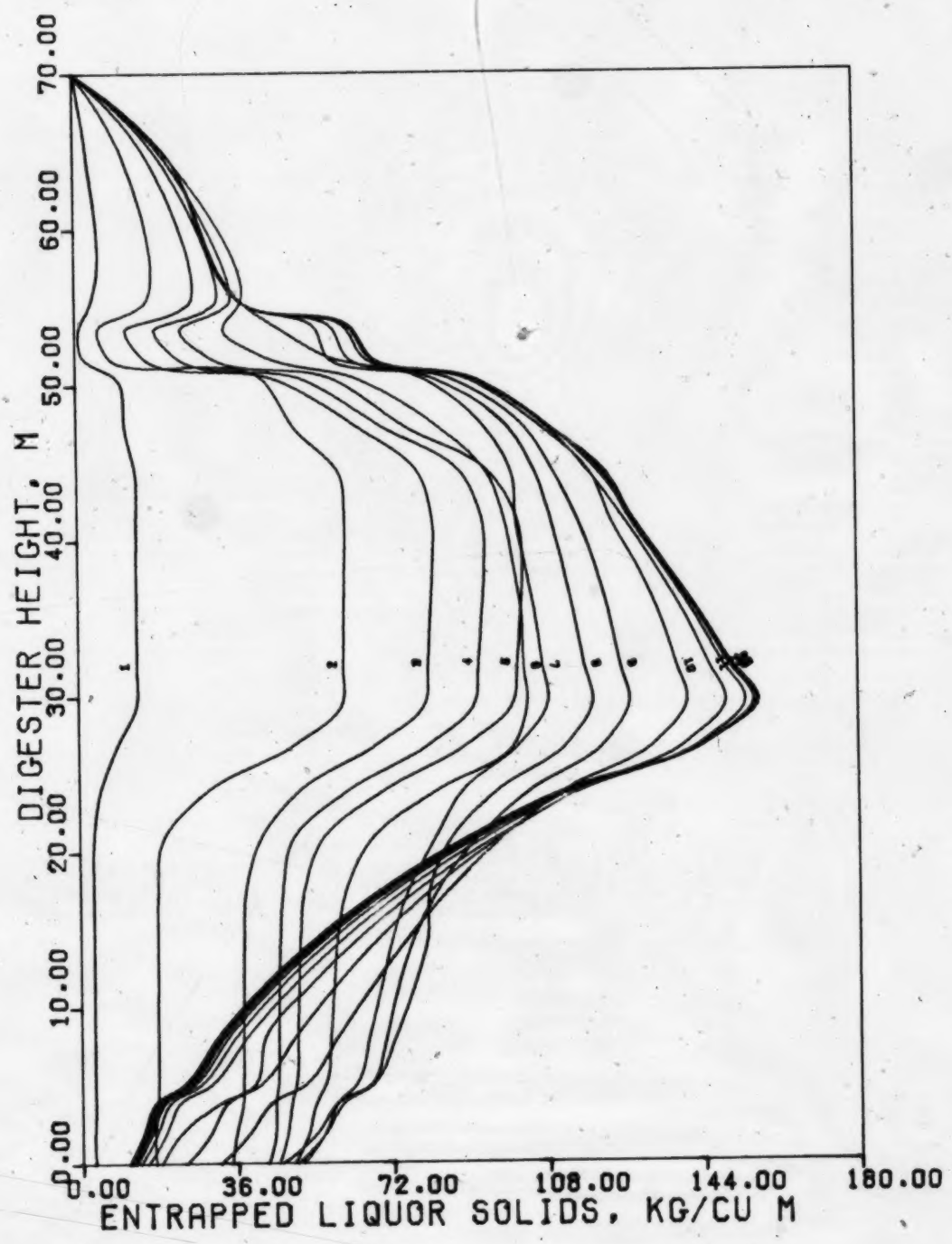


Figure 5.7 : Entrapped Liquor Solids Profiles for Run #1

heater at the exit is also apparent in the curves.

The 'history' curves for yield and lignin are plotted in Figures 5.9 and 5.10, these curves show the cooking conditions of the pulp leaving the digester at 900 minutes during its passage through the digester. The residence time for this set was about 400 minutes and the yield and lignin curves exhibit the same behavior as the earlier wood component profiles, Figures 5.1 and 5.2. There is some reaction in the impregnation zone followed by a steady drop through the heater and cooking zones. The reaction rate decreases sharply at the quench zone with a nearly zero rate in the wash zone, although the slight decrease in yield and lignin is still visible. The yield history curve when compared with the steady state profile of the same run (Figure 5.1) match closely except in the impregnation zone since the yield history curve includes only the major wood components and excludes the fast reacting acetyls, etc. while the instantaneous profiles calculate the 'true' yield.

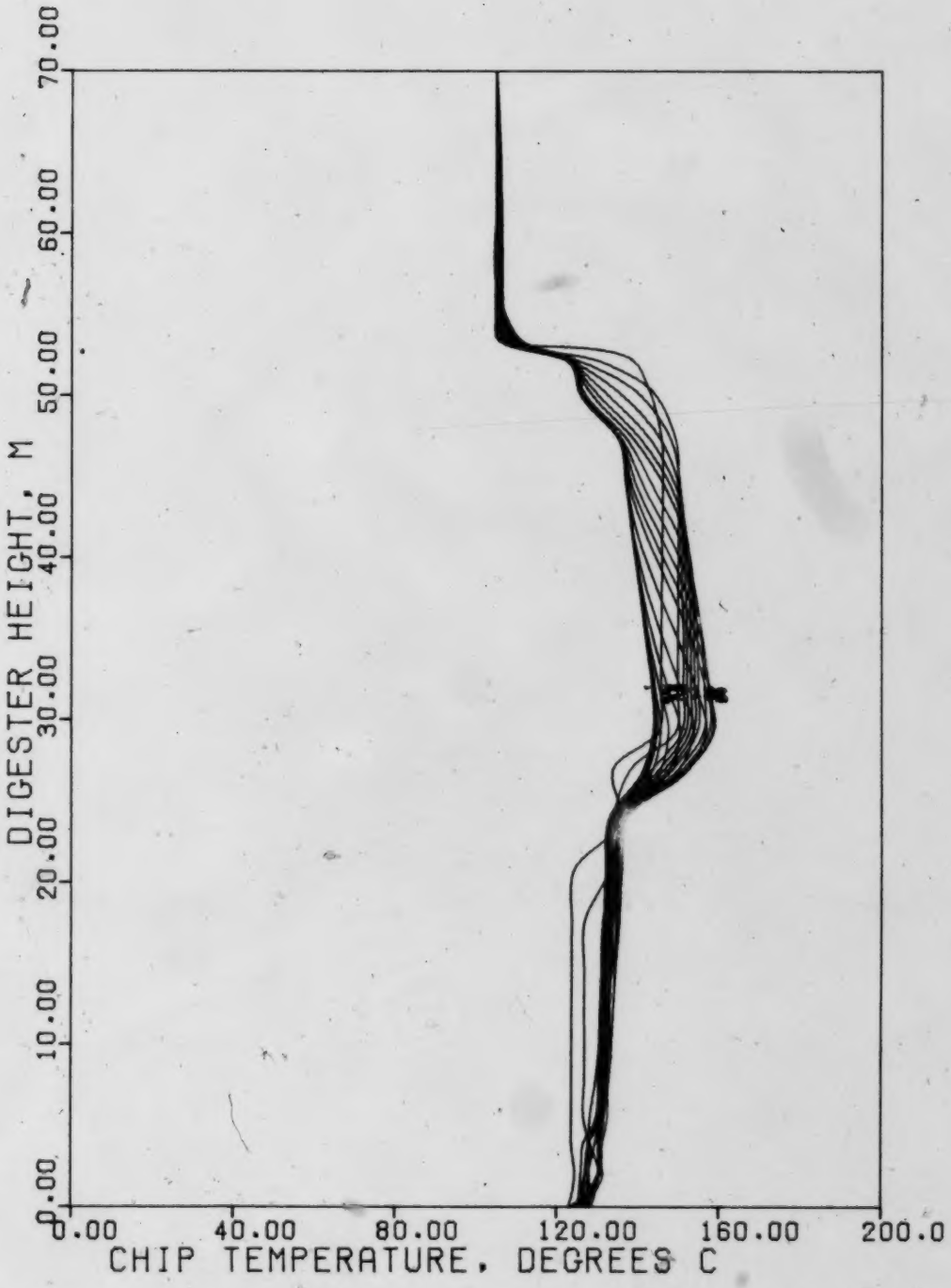


Figure 5.8 : Wood Chip Temperature Profiles for Run #1

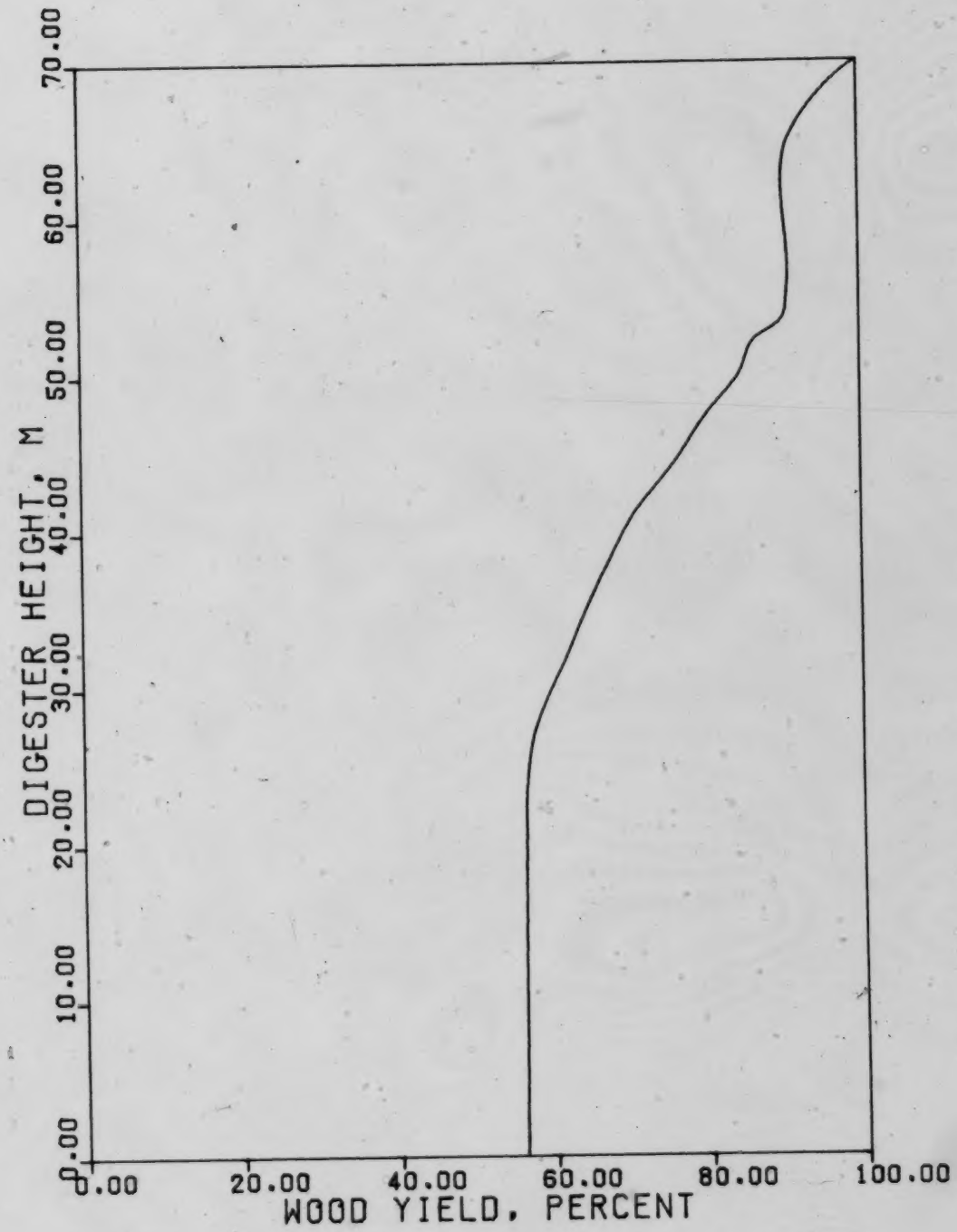


Figure 5.9 : Wood Yield History for Wood Exiting at 900 minutes for Run #1

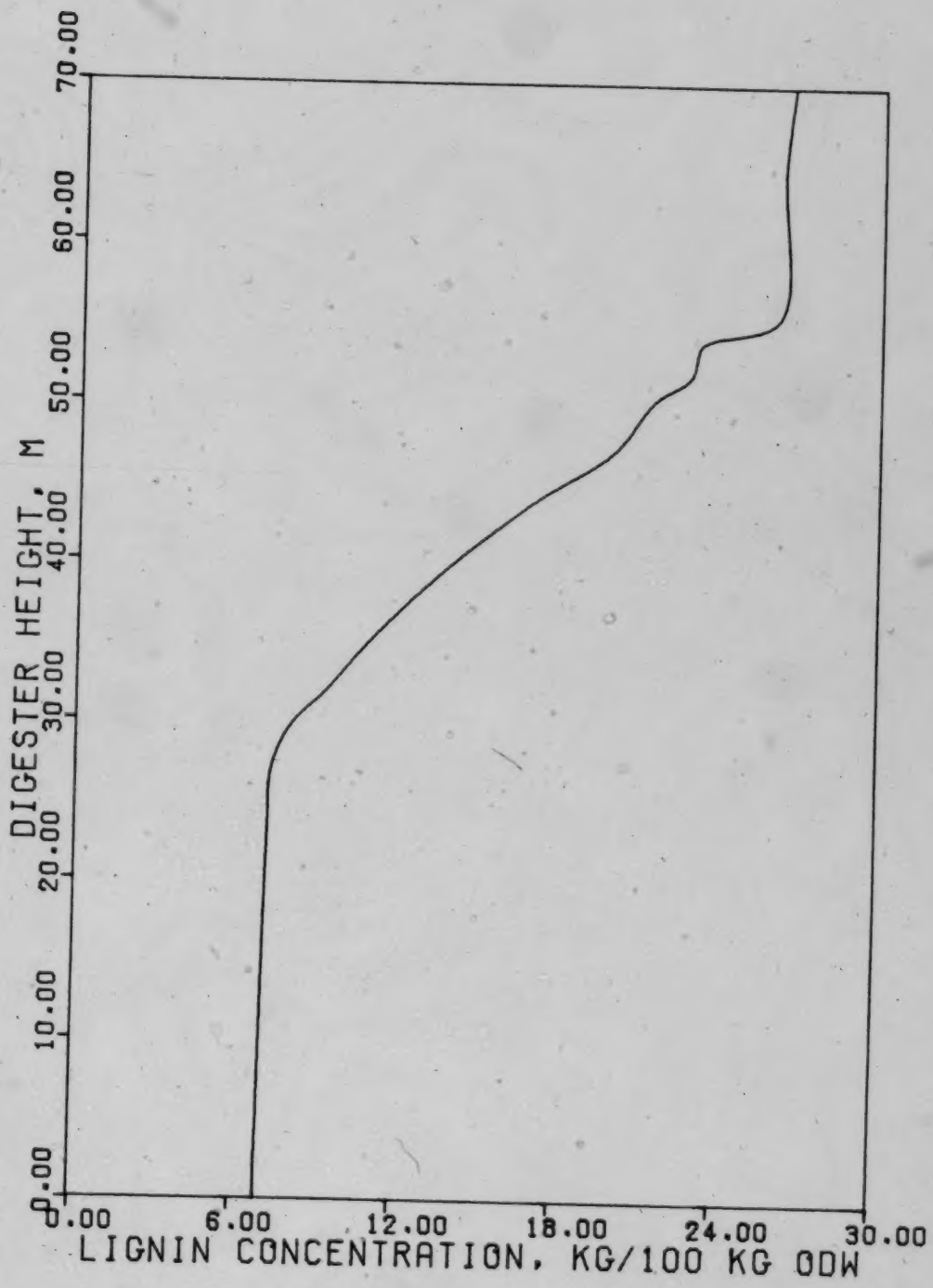


Figure 5.10 : Wood Lignin History for Wood Exiting at 900 minutes for Run #1

5.2 Alkali Concentration Change

An alkalinity change in the cooking liquor at the top of the digester is generally directly dependent on the operation of the chemical recovery cycle. Although this change can also be accomplished by varying the black liquor flow, this has its limitations since the black liquor flow is usually zero. The spent cooking liquor is recausticized to white liquor in the chemical recovery cycle and chemical losses are usually made up in the early part of the cycle. A step change in the alkalinity is hence usually made by direct hydroxide addition from a storage tank.

Step changes of ± 20% from the base steady state case were made to the white liquor alkalinity at the top of the digester. The ultimate response to this variation is a different rate of reaction and this effect is apparent from the blow line yield and the lignin content.

Figures 5.11 to 5.14 show the results for the alkali plus change. The yield at the blow line falls to 54% compared to 56% for the base case (Run #1) and the blow line Kappa number to 24.0 as opposed to 26.2. The steady state alkalinity in the chips increases and so does the residual solids at the extraction screen and in the final pulp.

For the negative step in alkali only yield and lignin concentrations are plotted as shown in Figures 5.15

and 5.16. The response for this case is in the reverse direction to that for the alkali plus change, as is expected. The yield and Kappa number values are higher and 58% and 29.1 respectively. The yield results obtained from the two alkali step changes give an estimate of the nonlinearities involved and also demonstrate that the H-Factor, which is a function of only cooking time and temperature would would not be an adequate variable for the control of the Kappa number in such cases.

5.3 Cooking Temperature Change

The main manipulated variable for the final product quality in the operation of the Kamyr digester in most mills is the cook zone temperature as set by the lower heater temperature. Increments as small as a quarter of a degree Celsius are used to adjust the digester operation. To study the effect of temperature, a step change of $\pm$ 5 ^{o}C was given to both the upper and lower heater temperatures from the base case. As with the alkali change, the heater temperature change ultimately increases the rate of reaction and the lignin and yield move in the same direction as with

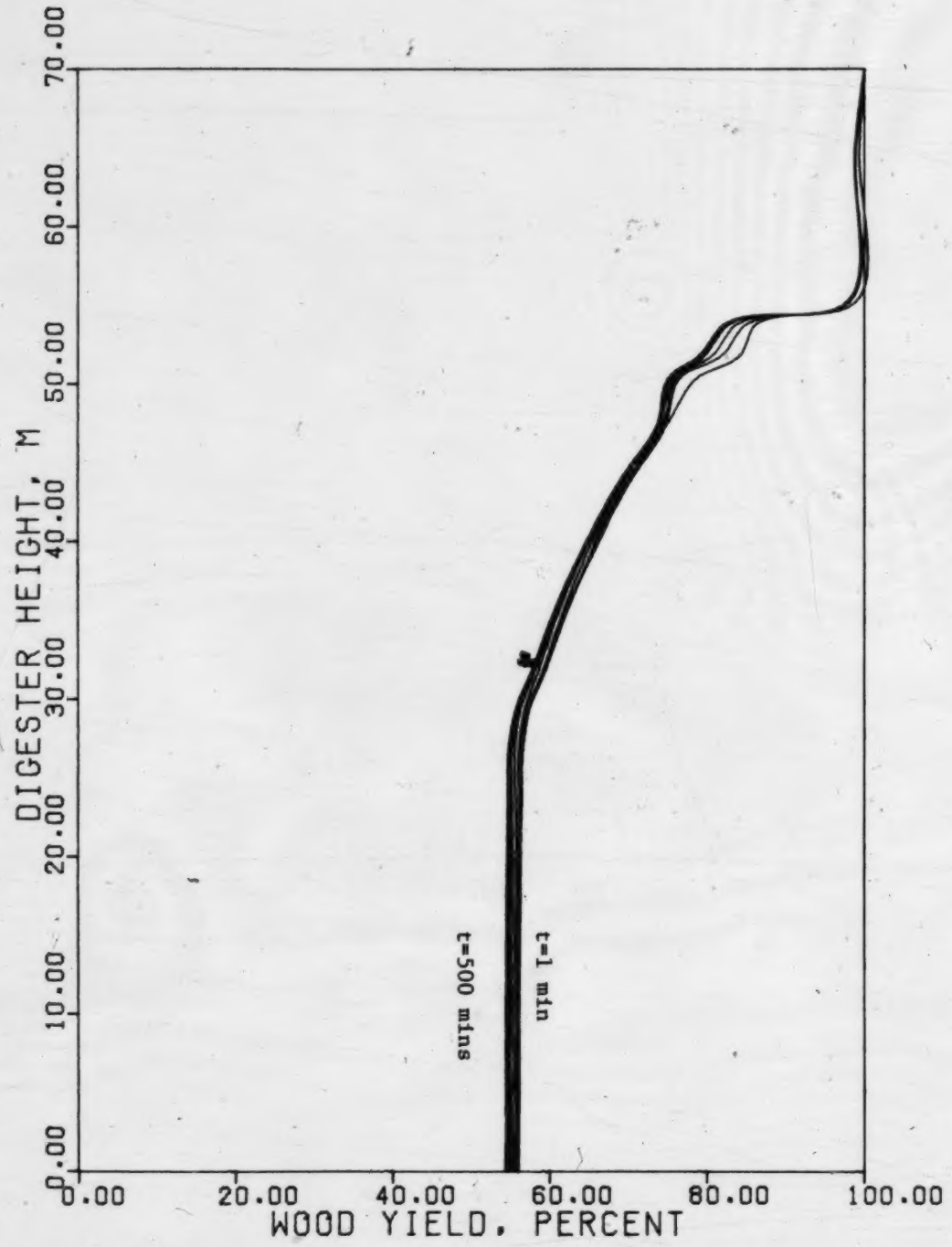


Figure 5.11 : Wood Yield Profiles for Run #2, a +20% Change in Alkali relative to the Base Case (Run #1)
(The profiles are at 1, 20, 50, 100, 150, 200, 250, 300, 350, 400, 450 and 500 minutes respectively)

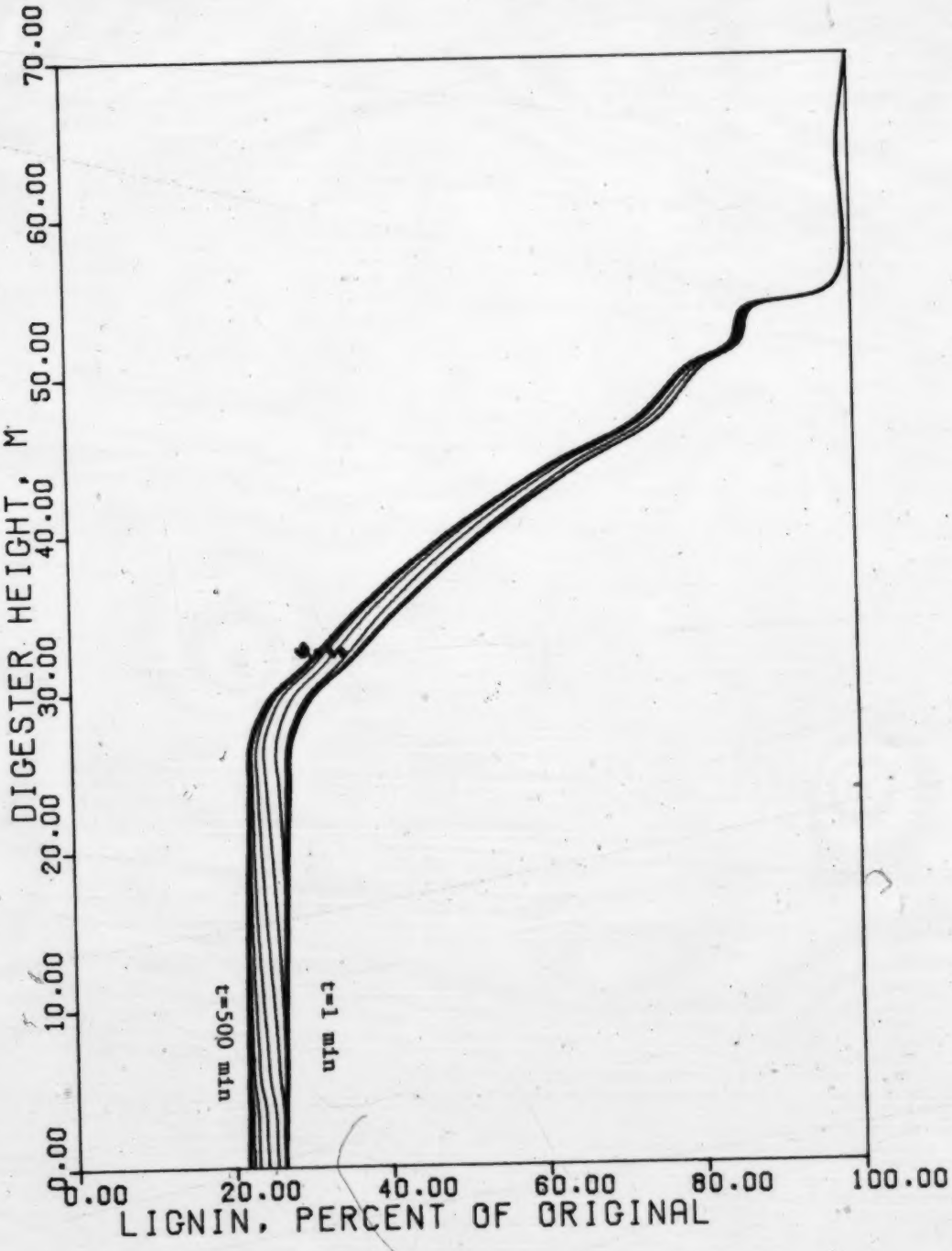


Figure 5.12 : Lignin Profiles for Run #2
(+20% Alkali Change)

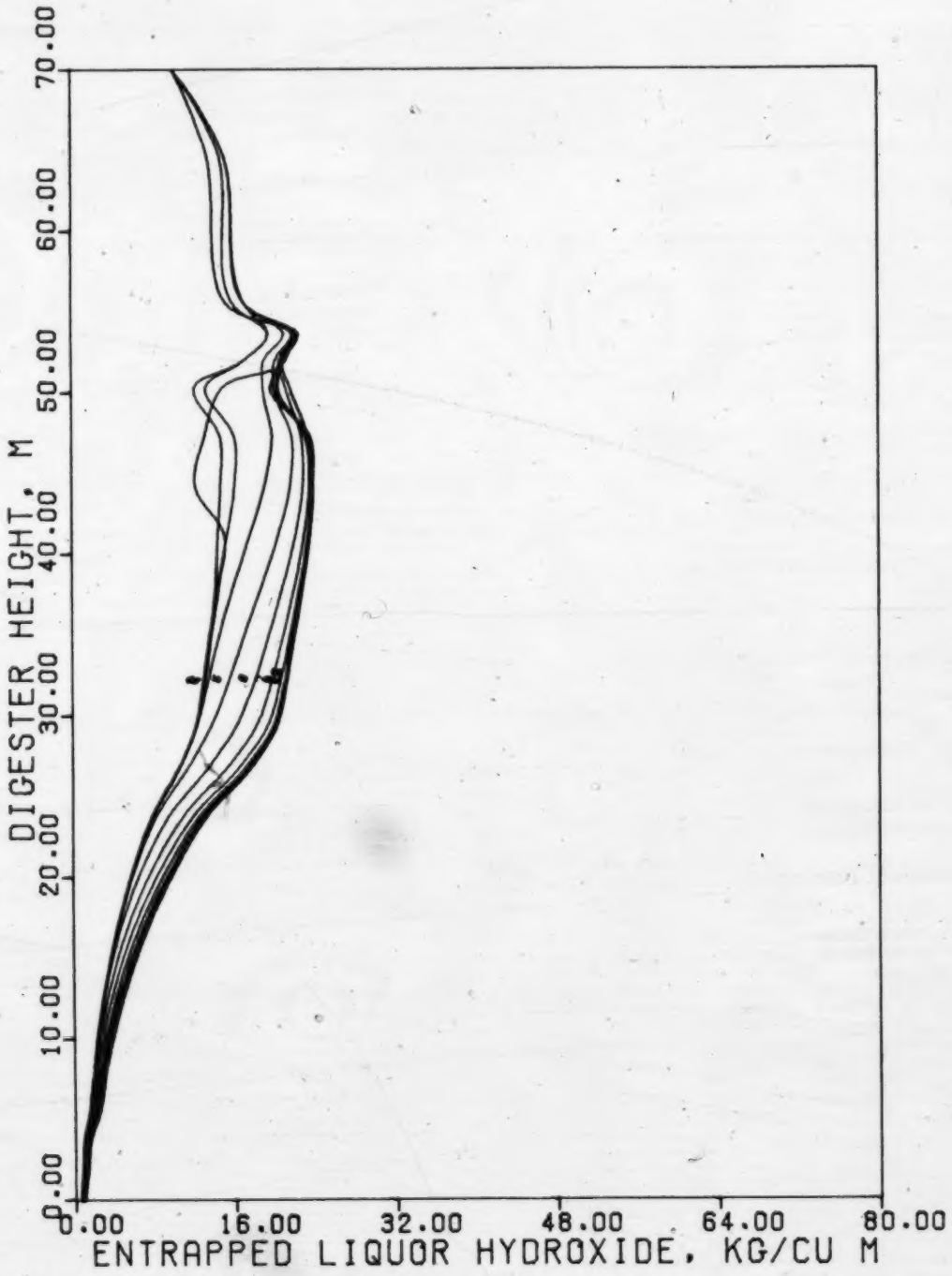


Figure 5.13 : Entrapped Liquor Hydroxide Profiles for Run #2 (+20% Alkali Change)

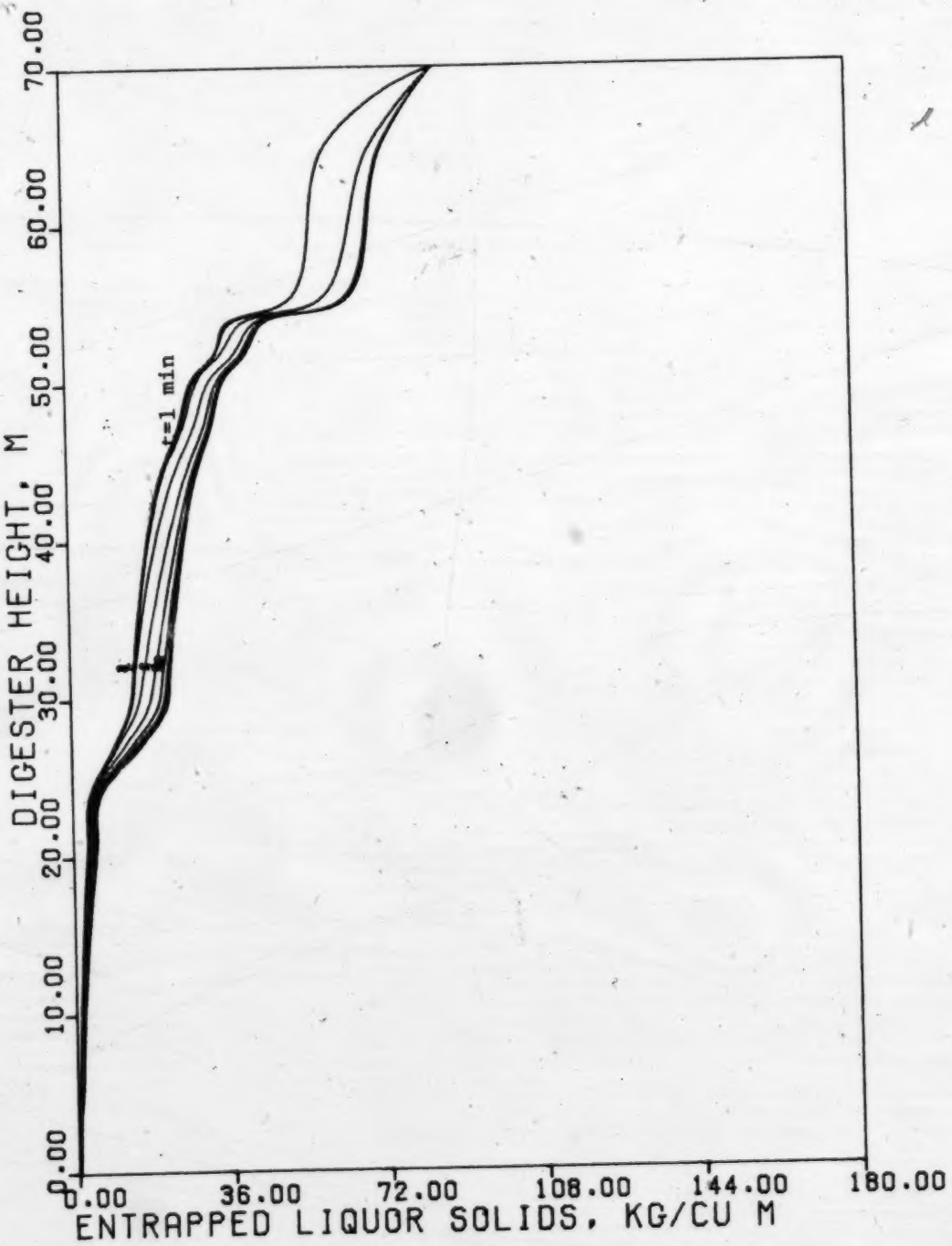


Figure 5.14 : Entrapped Liquor Solids Profiles for Run #2 (+20% Alkali Change)

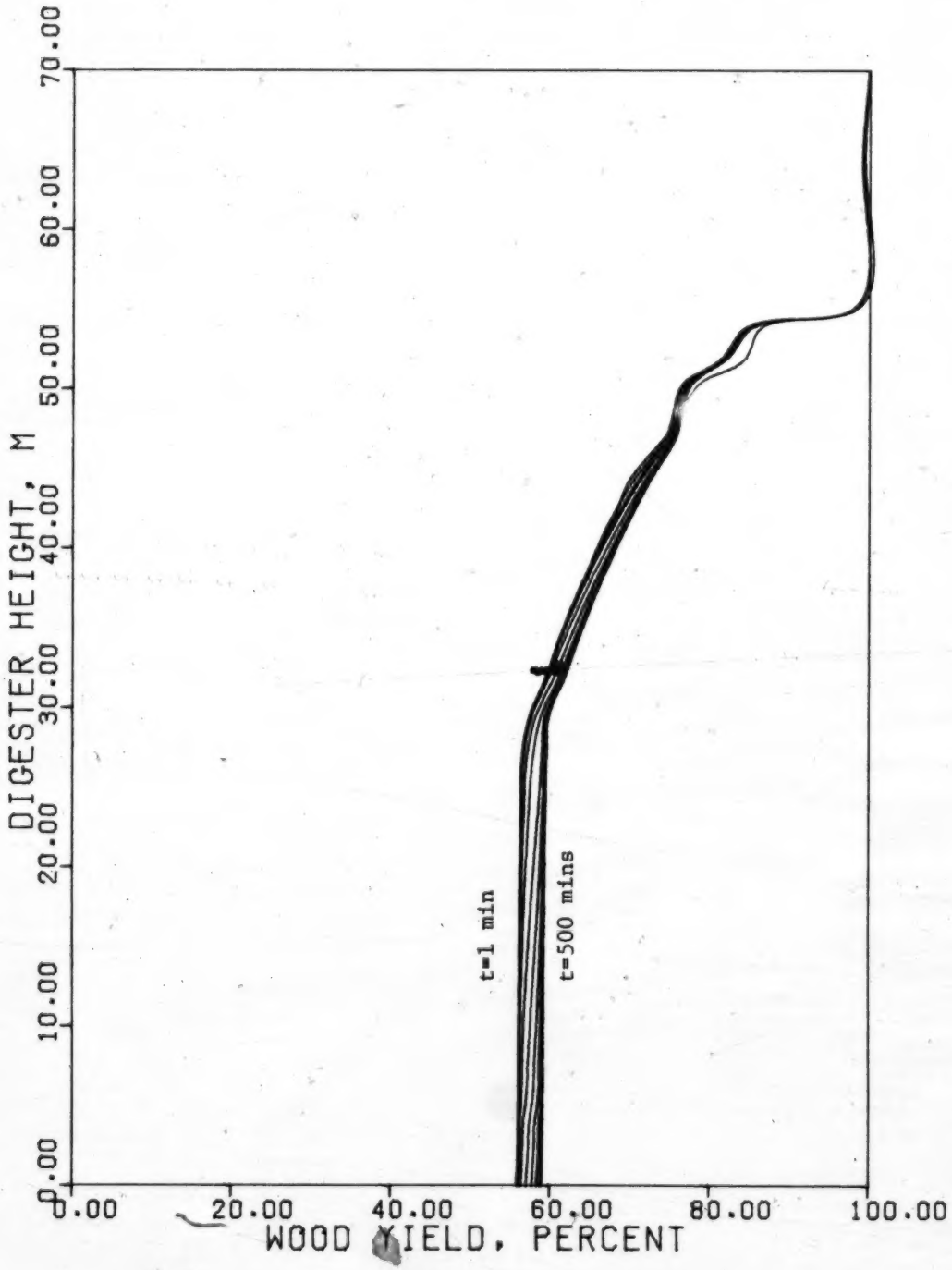


Figure 5.15 : **Wood Yield Profiles for Run #3, a -20% Alkali Change Relative to the Base Case (Run #1)** The profiles are plotted for the same times as in Run #2

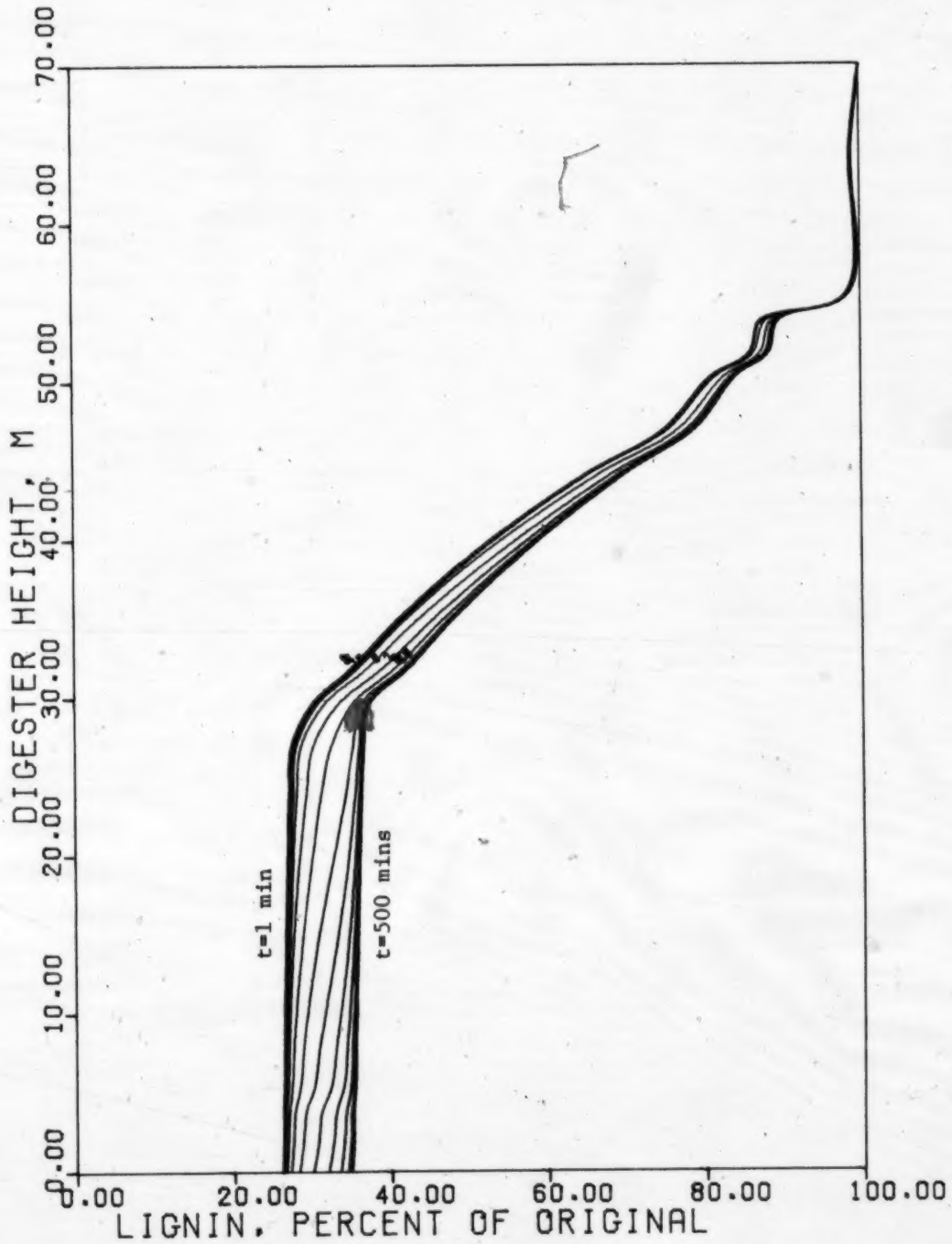


Figure 5.16 : Lignin Profiles for Run #3
(-20% Alkali Change)

the alkali changes. However, in this case the effect appears more quickly in the digester as the heater zones act below the impregnation zone whereas the alkali is introduced at the top of the digester.

The results from the step increase in temperature are shown in Figures 5.17 to 5.20. The yield and lignin are both lower than the starting base case as would be expected from a higher rate of reaction. The profiles for yield and lignin (Figures 5.17 and 5.18) are similar to the ones for Run #1 as the heater zones are the first affected and the temperature change then makes its way through the lower zones. The impregnation zone conditions are unchanged as the temperature of the streams entering the digester are the same as for the base case. The alkali concentration (Figure 5.19), which is initially the same as the steady state value for Run #1, is lower in the final steady state, as more chemicals have been used up to dissolve the wood components. The temperature response is plotted in Figure 5.20. For the 5 ^{o}C step down the reaction rates are lower and hence more wood and lignin appear in the blow line. These results are plotted in Figures 5.21 and 5.22 respectively. The step change in the heater temperatures gave a Kappa number and

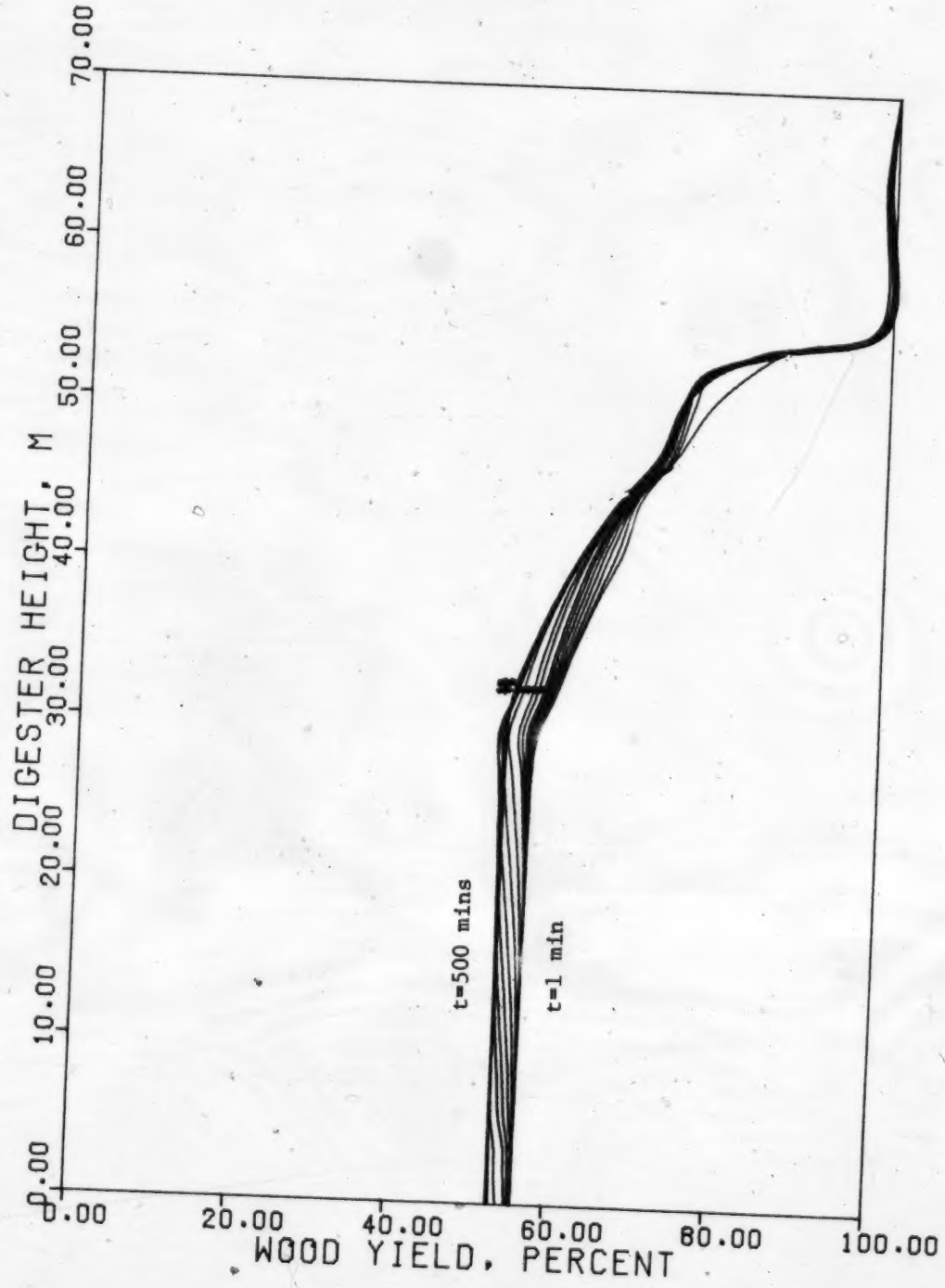


Figure 5.17 : Wood Yield Profiles for Run #4, a +5 degree C Change in Temperature Relative to the Base Case

(The profiles are at 1, 5, 10, 15, 20, 25, 30, 40, 50, 75, 100, 125, 150, 175, 200, 300, 350, 400, 450 and 500 minutes respectively)

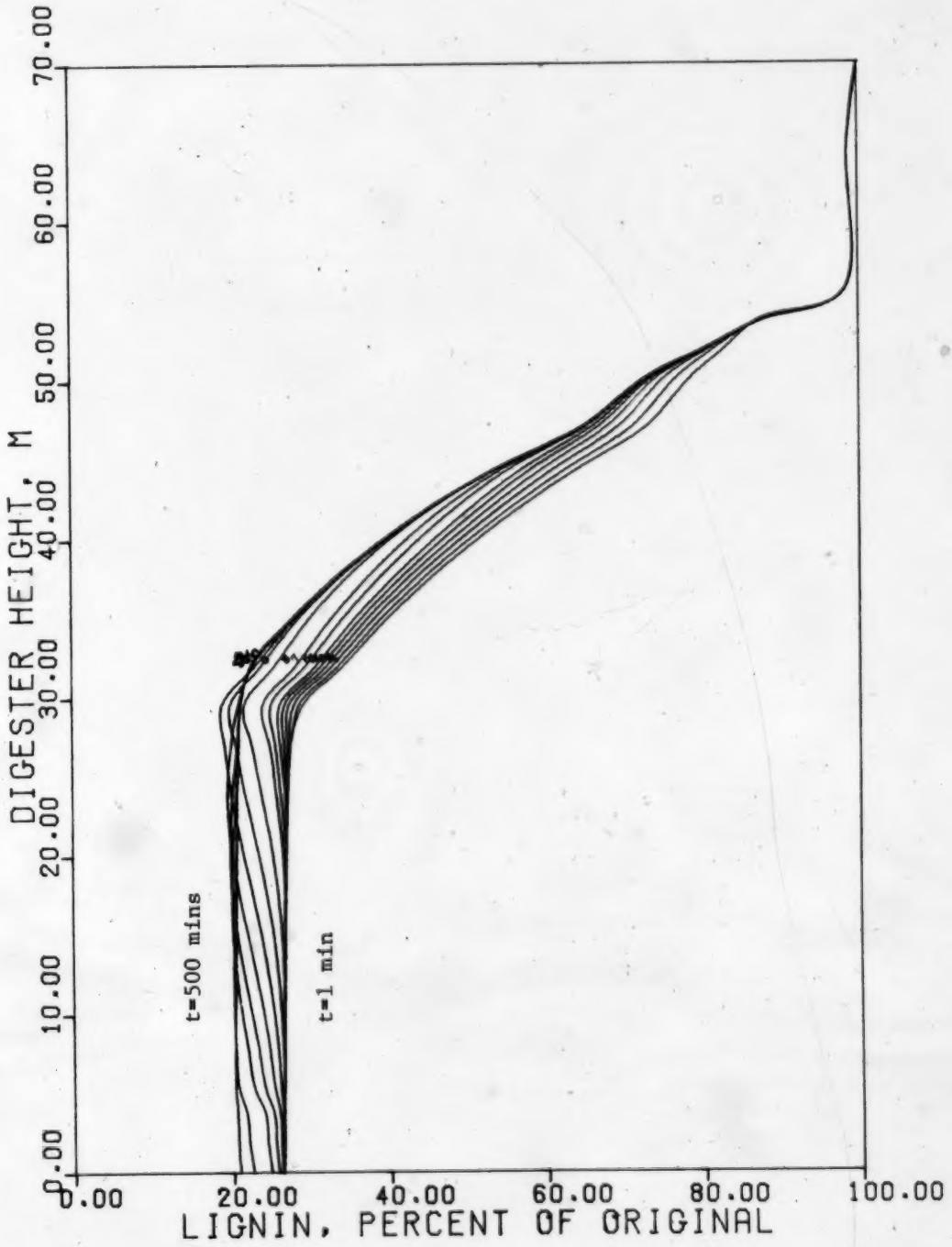


Figure 5.18 : Lignin Profiles for Run #4
(+5 degree C Temperature Change)

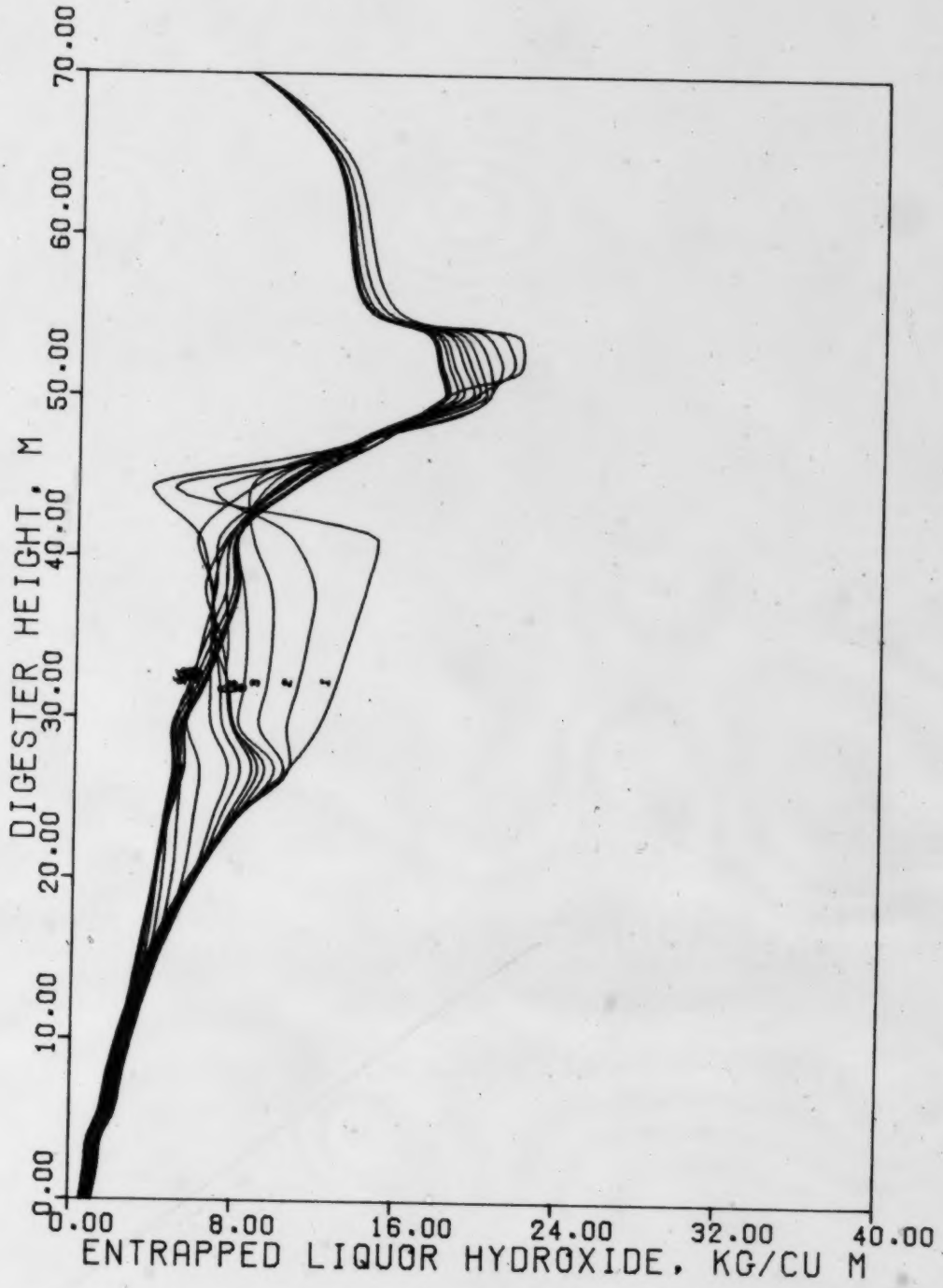


Figure 5.19 : Entrapped Liquor Hydroxide Profiles for Run #4, (+5 degree C Temperature Change)

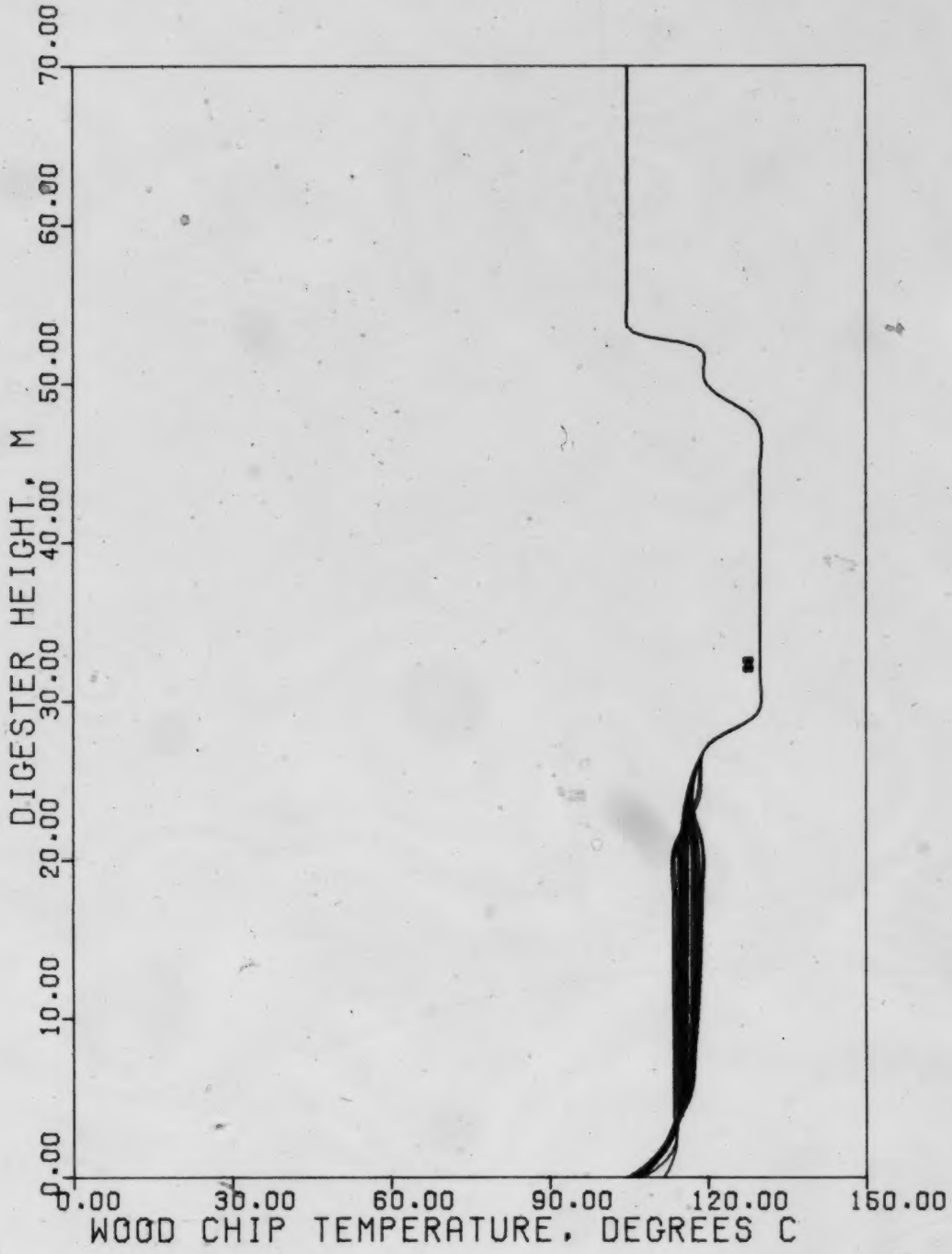


Figure 5.20 : Wood Chip Temperature Profiles for Run #4
(+5 degree C Temperature Change)

wood yield of 22.6 and 52% for the plus change and values of 31.0 and 60% for the temperature minus change. These temperature changes are only about ± 2% of the cooking zone temperature but the difference in the yield and lignin content is higher than that for the alkali changes which were approximately ± 20%. This provides sufficient justification for using temperature to control the final pulp quality in industry since chemicals are more expensive and have less effect on the final product quality.

5.4 Cooking Zone Length Variation

The variation of cooking zone length has the same effect as changing the retention time in the cook zone. This may have to be done in cases where the pulp is not fully cooked in the cook zone or where the pulp specifications have to be changed without changing either the production rate, temperature or the alkalinity. The length of the cook zone would be shortest for a 'hard' cook where the upper heater is shut off and the lower heater is set to the maximum possible under the circumstances. The pulp is then given a cold quench that cuts off the reaction

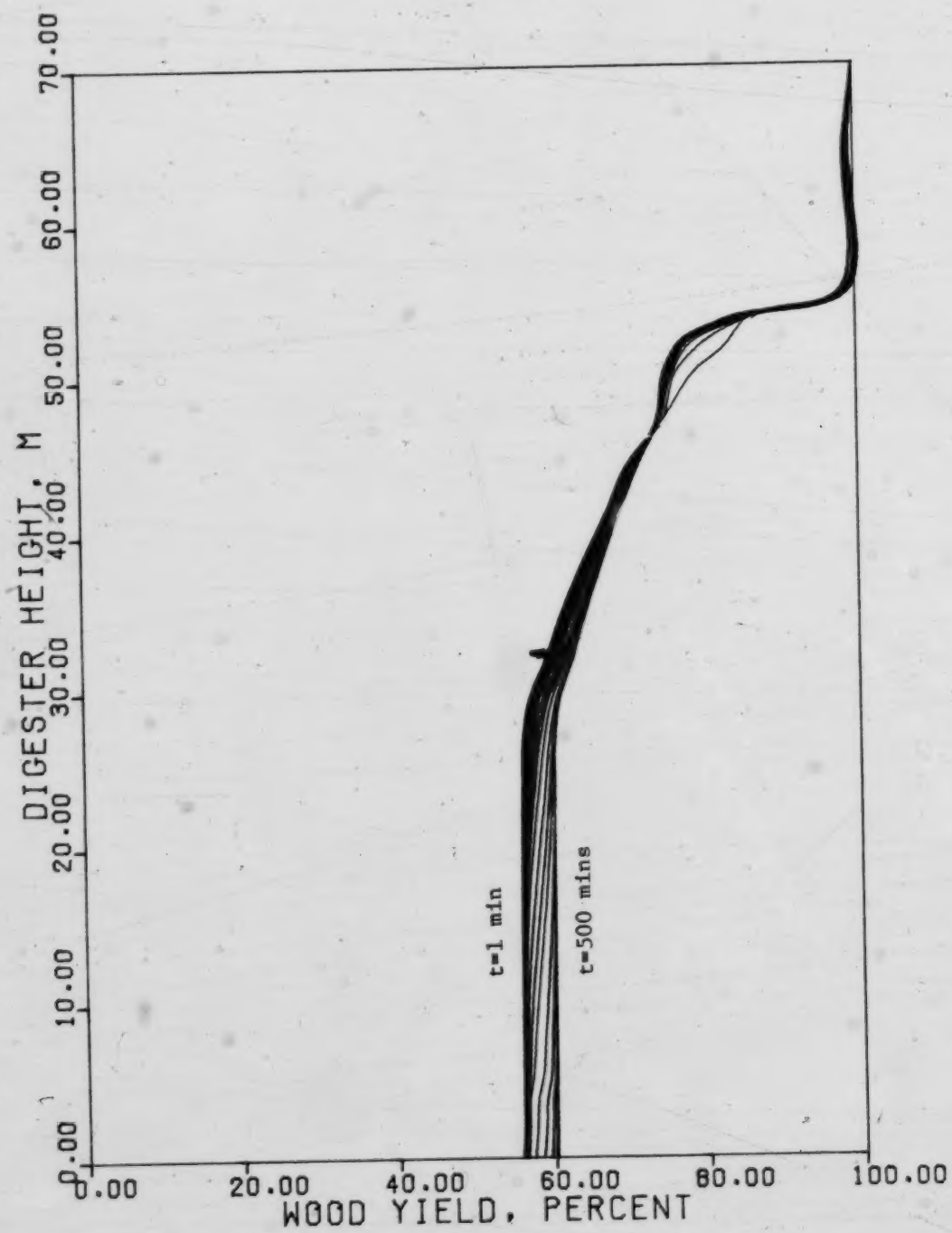


Figure 5.21 : Wood Yield Profiles for Run #5, a -5 degree C Temperature Change Relative to the Base Case (Run #1)

The profiles are at the same times as in Run #4

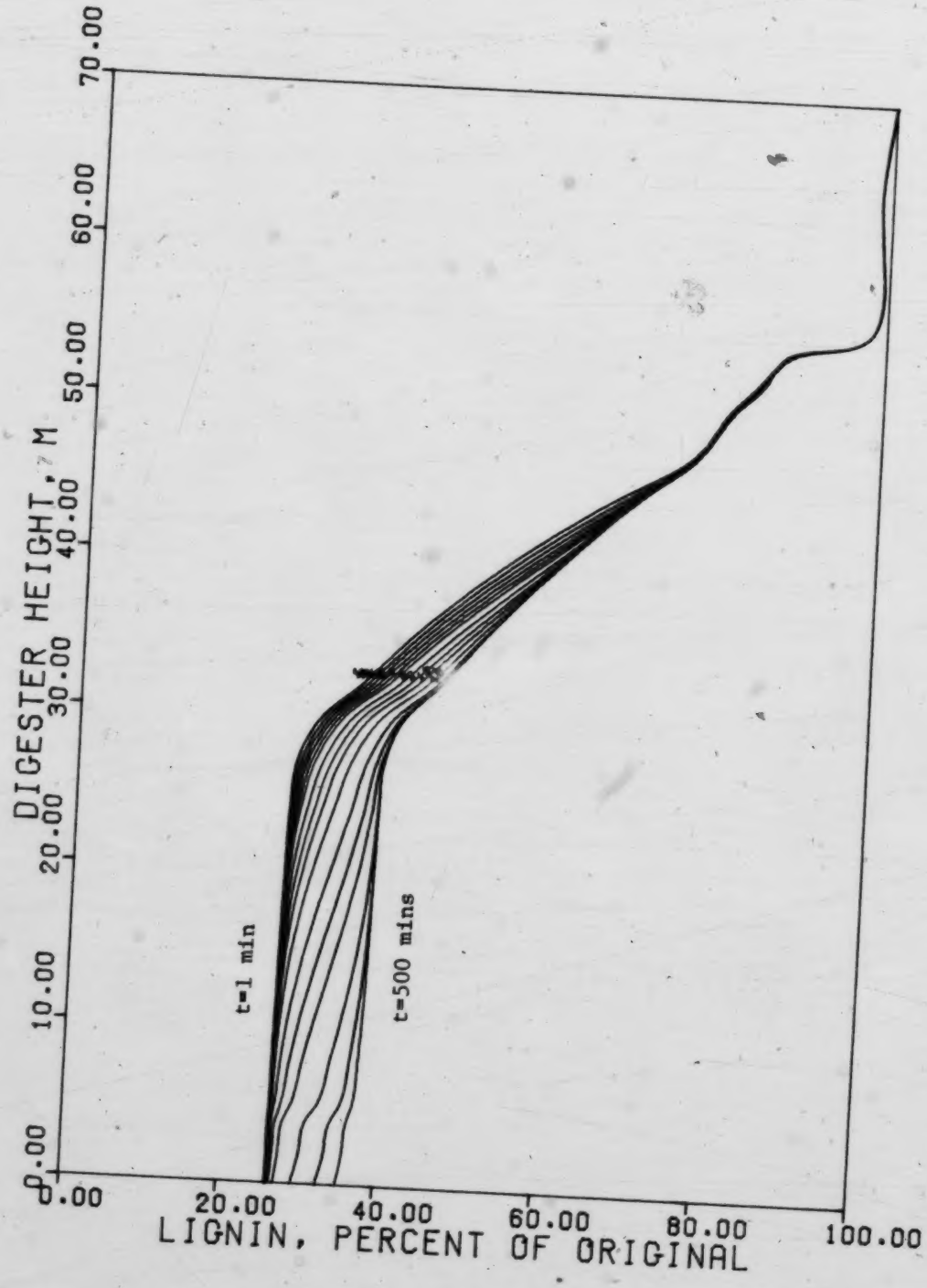


Figure 5.22 : Lignin Profiles for Run #5
(-5 degree C Temperature Change)

completely at the quench/extraction zones. Similarly the length would be longest for a 'soft' cook where both heaters are operating at below their capacity and there is little quenching, which allows the reaction to proceed into the wash zone. In this case the length of the cook zone is dependent upon the extraction rate and the washing temperature.

The 'hard' cook was illustrated by shutting off the upper heater and raising the temperature of the lower heater by 15 ^{o}C. The chips were allowed to cook at this temperature and quenched with a stream at about the same temperature as for the cold blow. This was done by not recycling quench liquor from the extraction screen and using only the 'cheater' flow. This cut off the reaction almost completely and hence there was limited cooking in the wash zone. The yield and lignin curves are given in Figures 5.23 and 5.24 respectively. The yield and Kappa numbers in the blow line were 58% and 28.0 . The entrapped liquor hydroxide and the temperature are plotted in Figures 5.25 and 5.26.

The soft cook was with the upper and lower heaters at ten degrees below the base level, and the quench flow

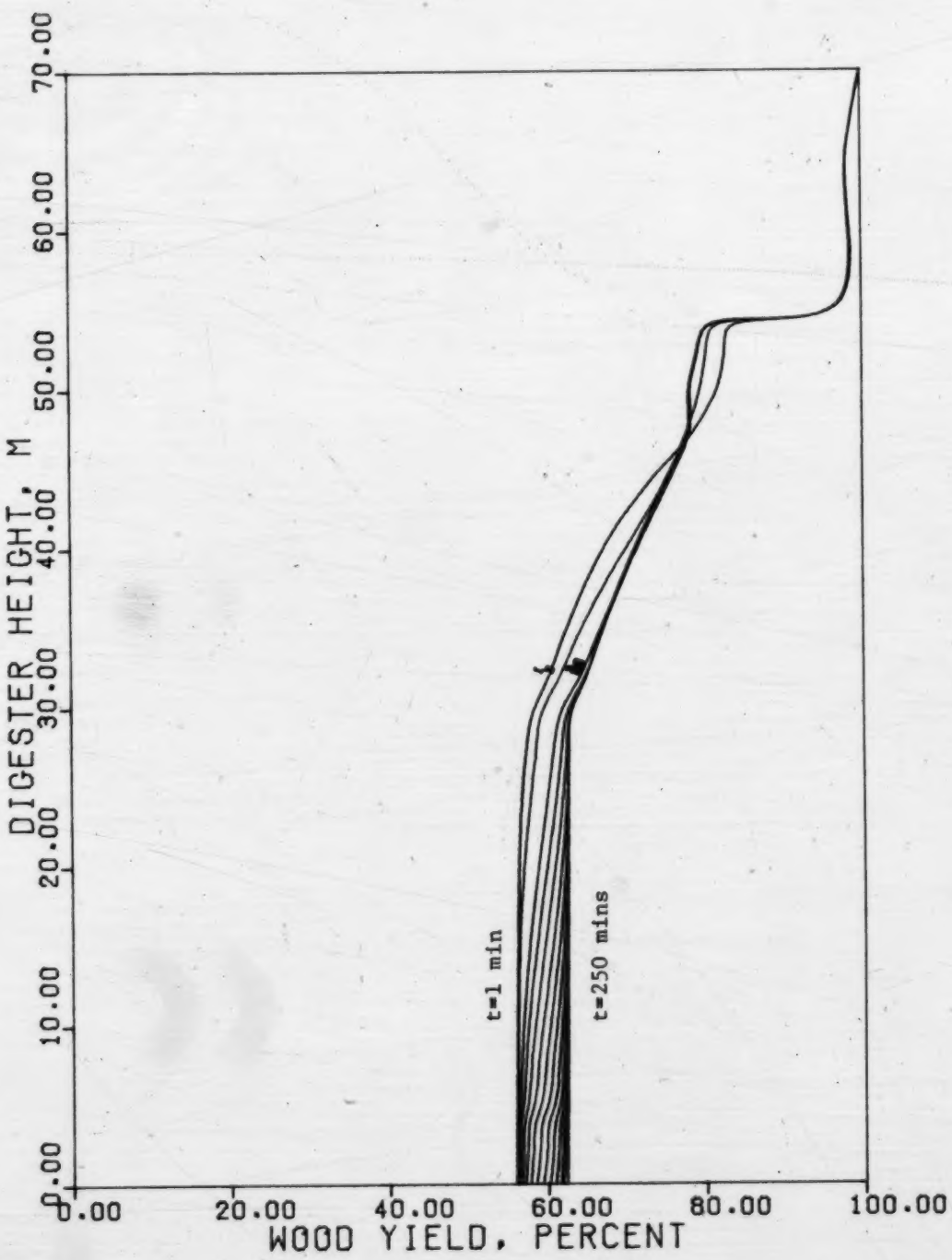


Figure 5.23 : Wood Yield Profiles for Run #6, a Hard Cook of Chips, High Lower Heater Temperature and Cold Quench

(These profiles are at 1, 10, 20, 30, 50, 75, 100, 125, 150, 175, 200, 225 and 250 minutes respectively)

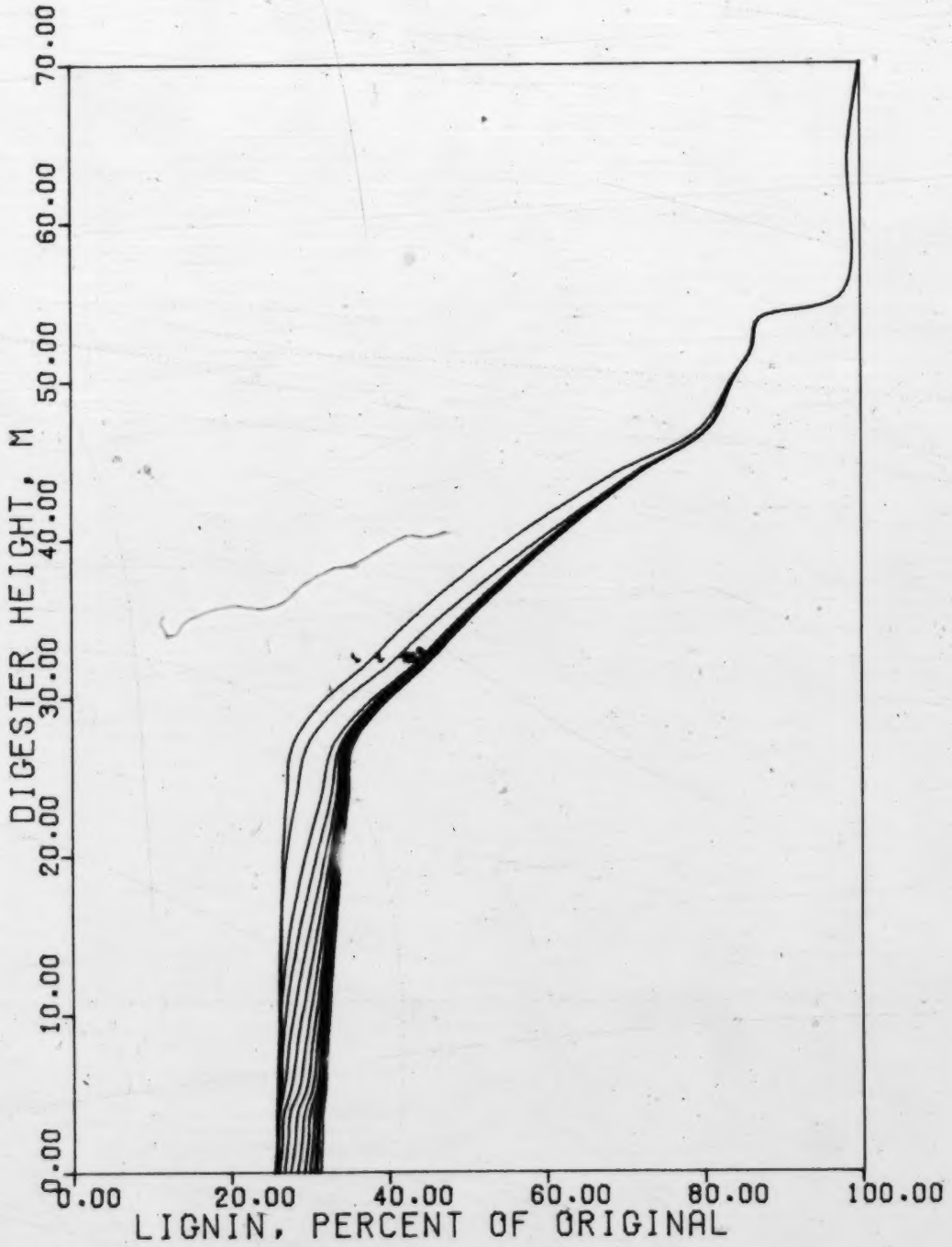


Figure 5.24 : Lignin Profiles for Run #6,
(Hard Cook of Chips)

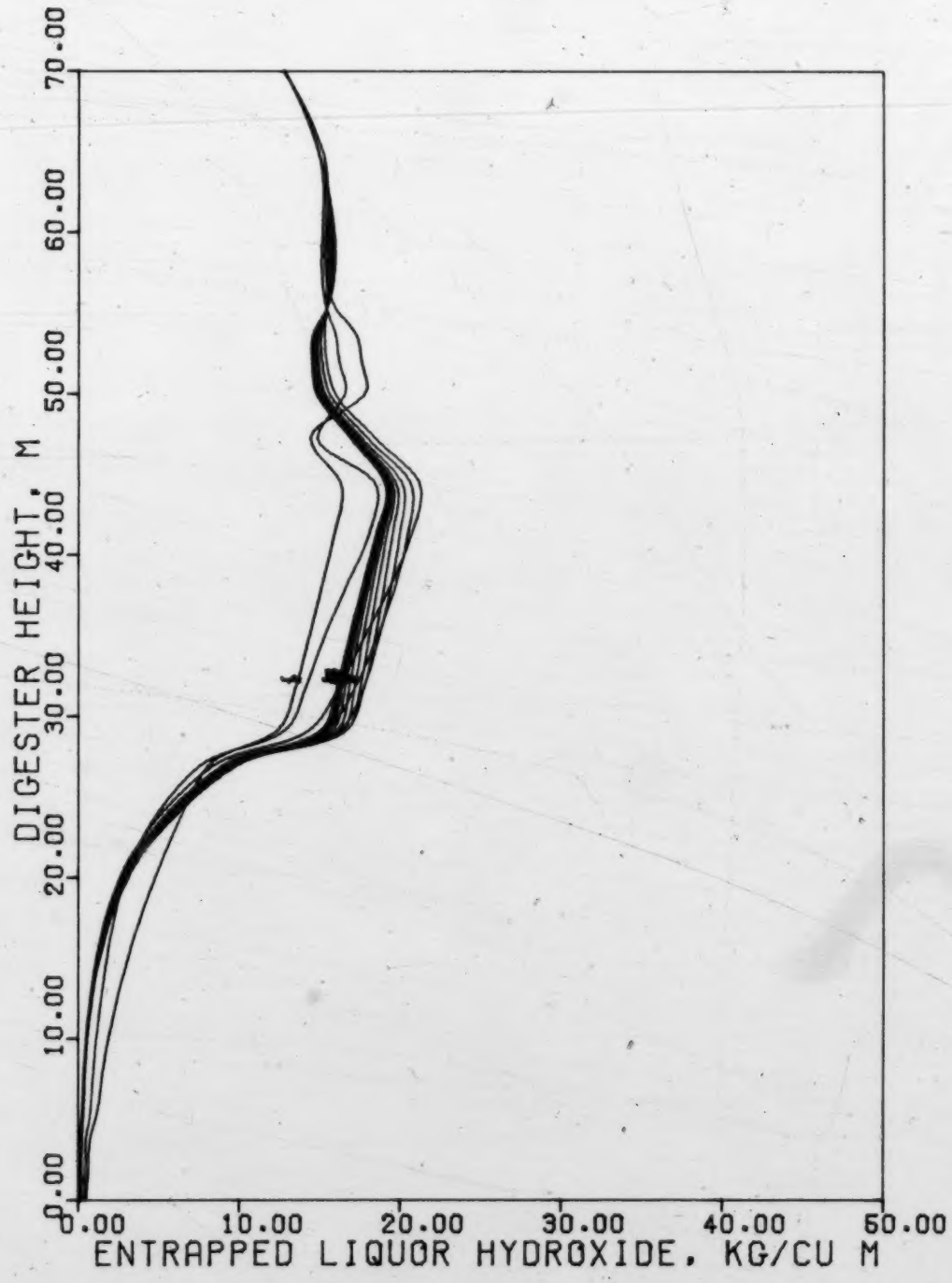


Figure 5.25 : Entrapped Liquor Hydroxide Profiles for Run #6, (Hard Cook of Chips)

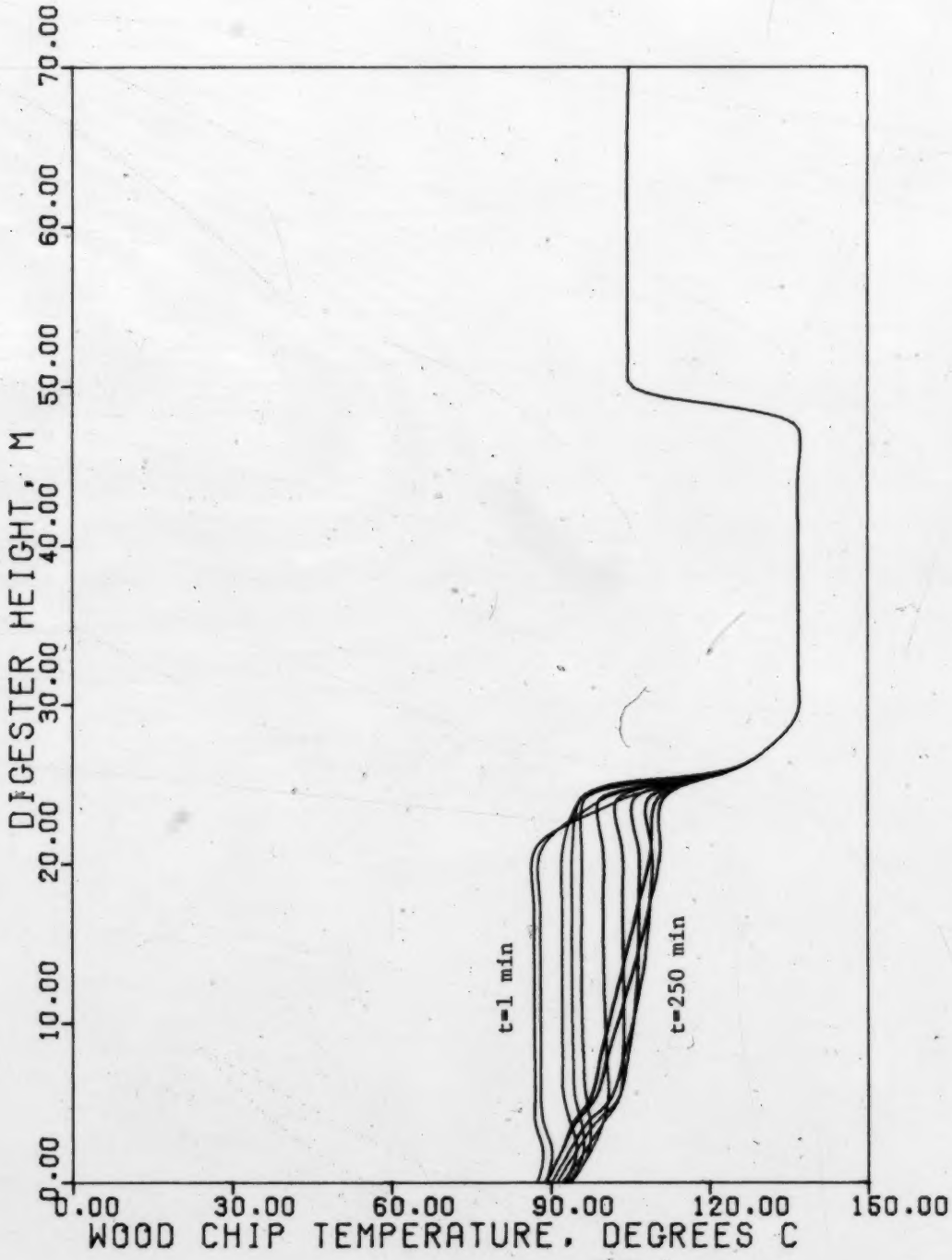


Figure 5.26 : Chip Temperature Profiles for Run #6
(Hard Cook of Chips)

shut off completely to allow cooking to proceed into the wash zone. The results for yield, lignin, entrapped liquor hydroxide and chip temperature are shown in Figures 5.27 to 5.30. The yield for this case is 62% and the Kappa number is 32.0 . The concentration of entrapped liquor in the pulp is higher than normal and further washing would have to be done before the pulp could be used further downstream in the mill.

The results from the cook zone length variation runs show that the pulp quality is dependent on the cooking temperature profile that the chips have been subjected to. The results also show that although the Kappa numbers are approximately equal, the yields are not and neither are the Kappa numbers. The K-number control scheme and the H-Factor scheme would both have difficulties in predicting the final product specifications.

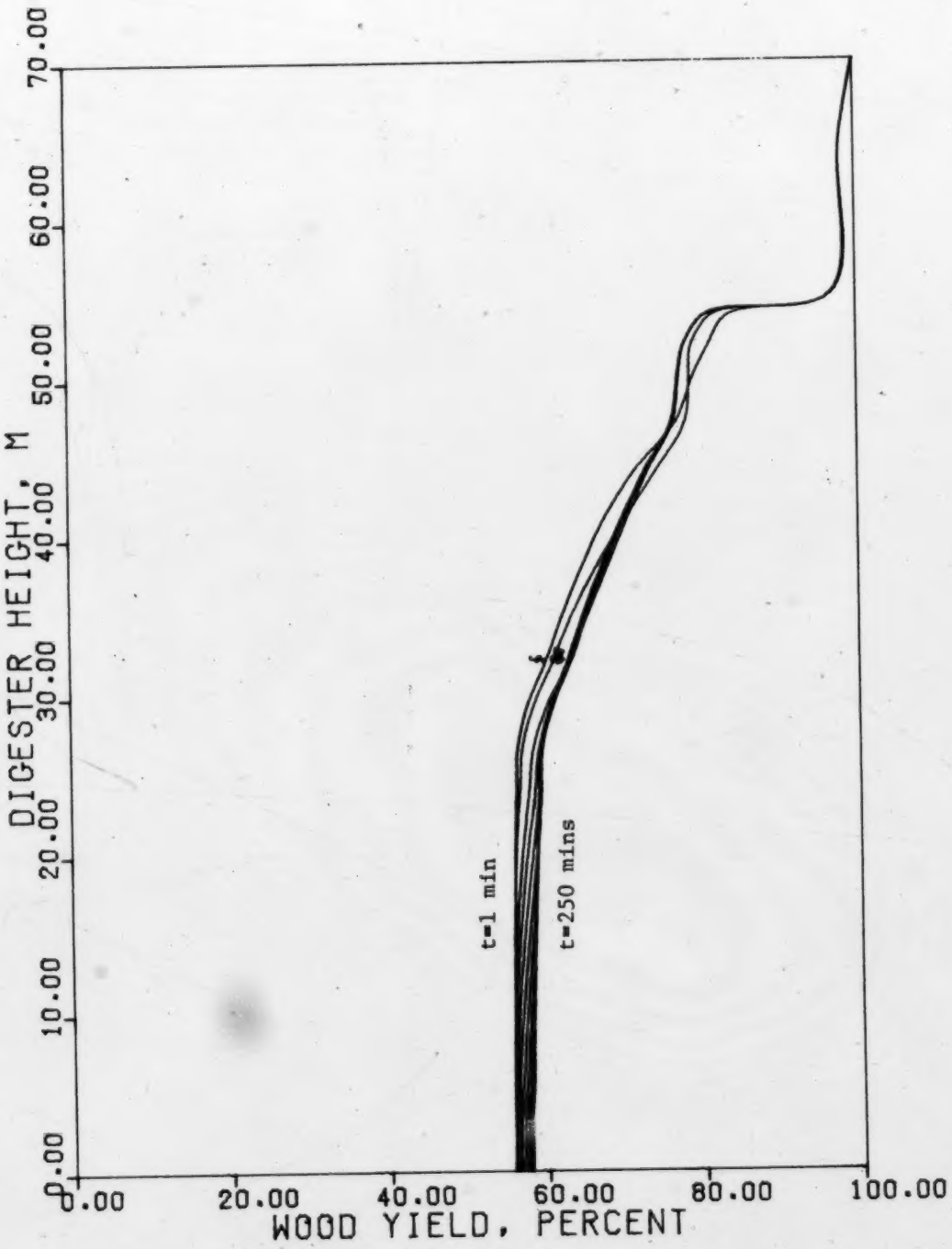


Figure 5.27 : Wood Yield Profiles for Run #7, a Soft Cook of Chips, Low Heater Temperatures and Warm Quench to Allow Cooking in the Wash Zone

These profiles are at the same times as in Run #6

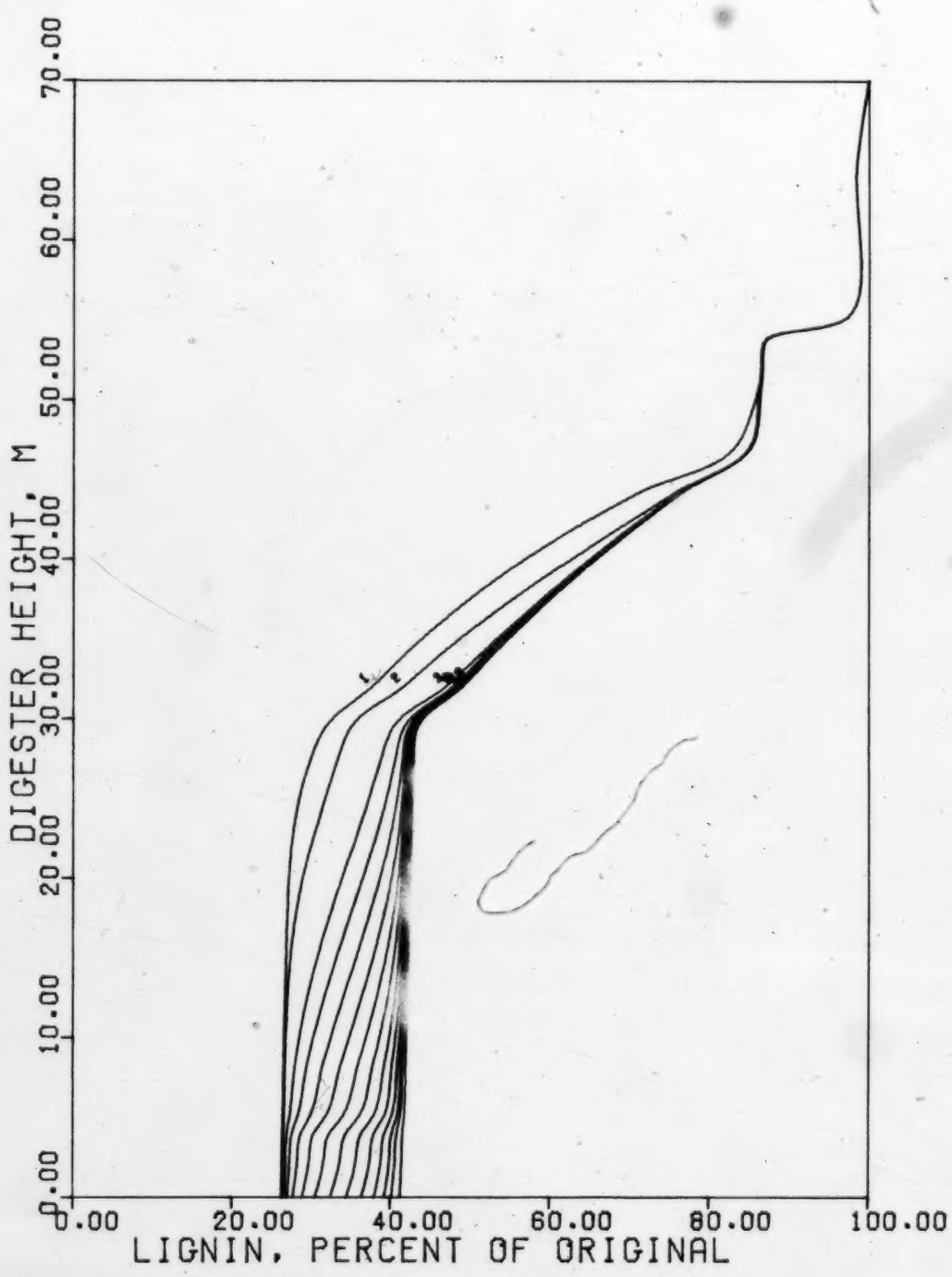


Figure 5.28 : Lignin Profiles for Run #7, (Soft Cook of Chips)

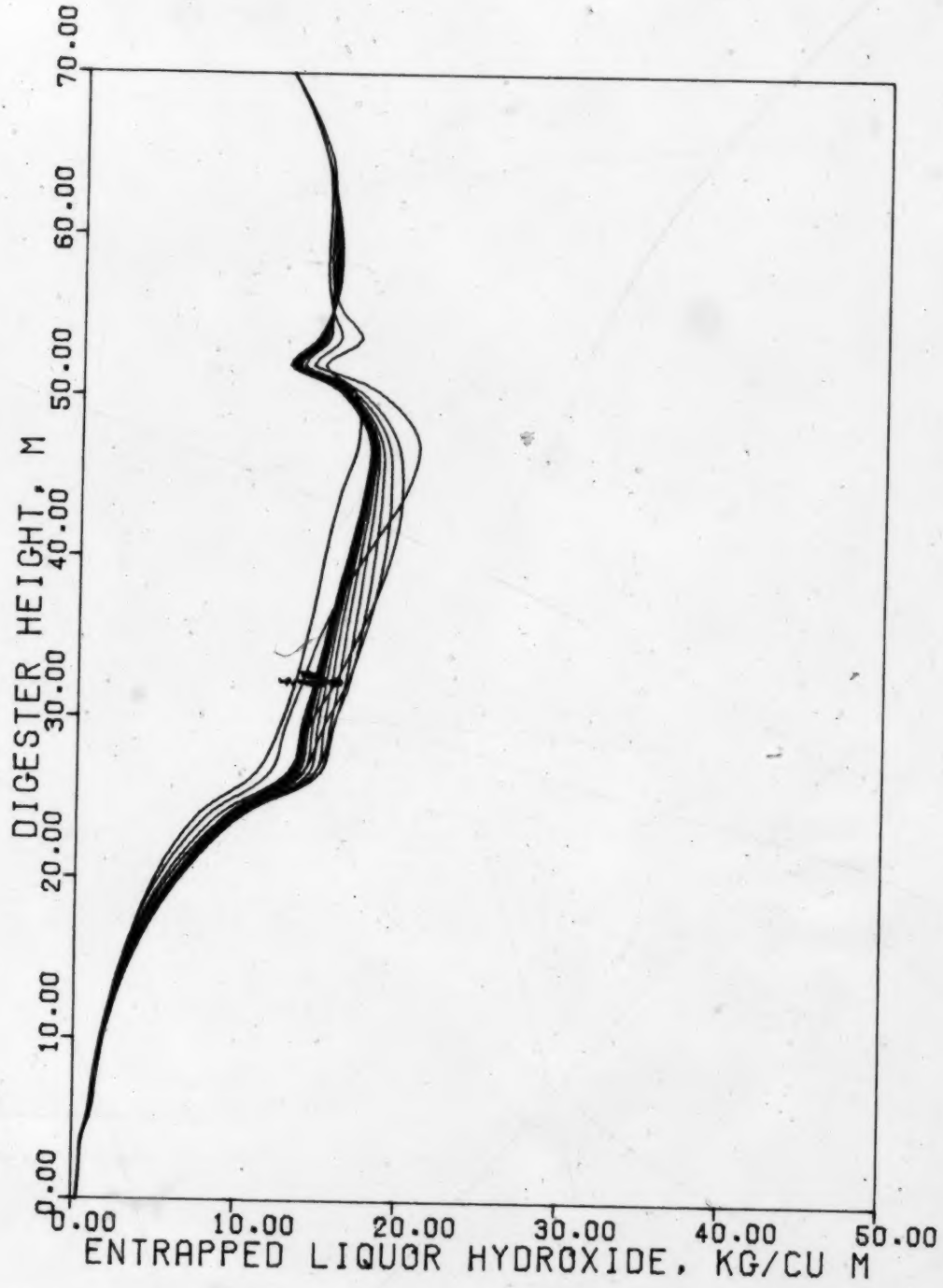


Figure 5.29 : Entrapped Liquor Hydroxide Profiles for Run # 7, (Soft Cook of Chips)

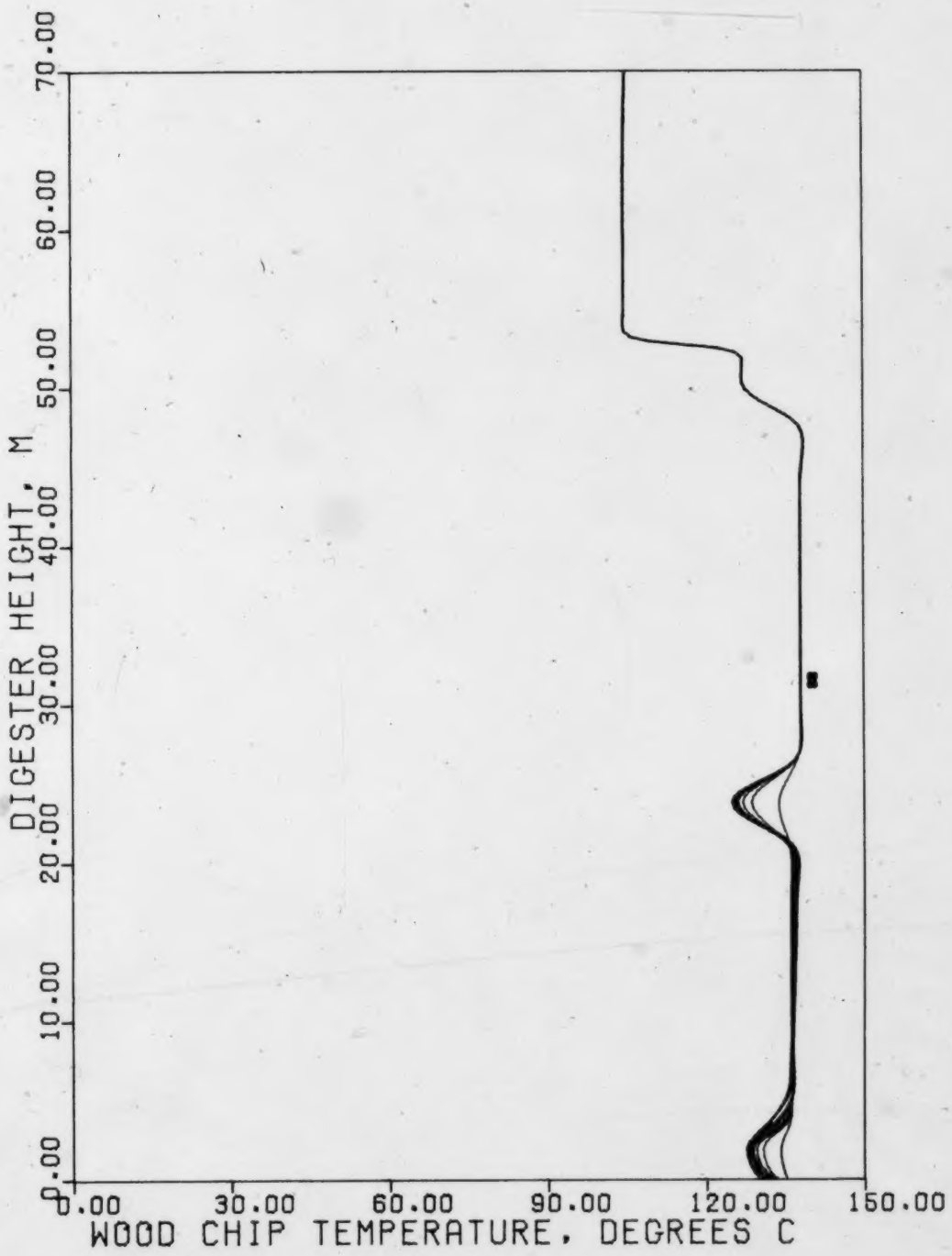


Figure 5.30 : Chip Temperature Profiles for Run #7
(Soft Cook of Chips)

5.5 Production and Grade Changes

The production rate and grade changes have a requirement for more or less chemicals and/or heater temperatures depending on the direction of the change. The Kappa number and yield would therefore be significantly different if the conditions were left unadjusted. The production change creates a different cook zone retention time and either of the three alternatives discussed earlier could be used to adjust the final pulp quality. A grade change is different than a production rate change since the product specifications have changed and the object is minimum off-grade pulp. A production rate change was tried by making a +10% step change in chip flow rate relative to the base condition. The results for yield and lignin are shown in Figures 5.32 and 5.33 and have, as expected, a higher pulp yield and Kappa number.

5.6 Species Change

A species change is accompanied by a different bulk

density and different reaction rate constants. A species change from hardwood to softwood was tried from base case conditions and the pulp tracked through the digester. The lignin and yield transient profiles are shown in Figures 5.33 and 5.34. Hardwood has a faster reaction rate than softwood and at steady state a lower yield and Kappa number value is observed.

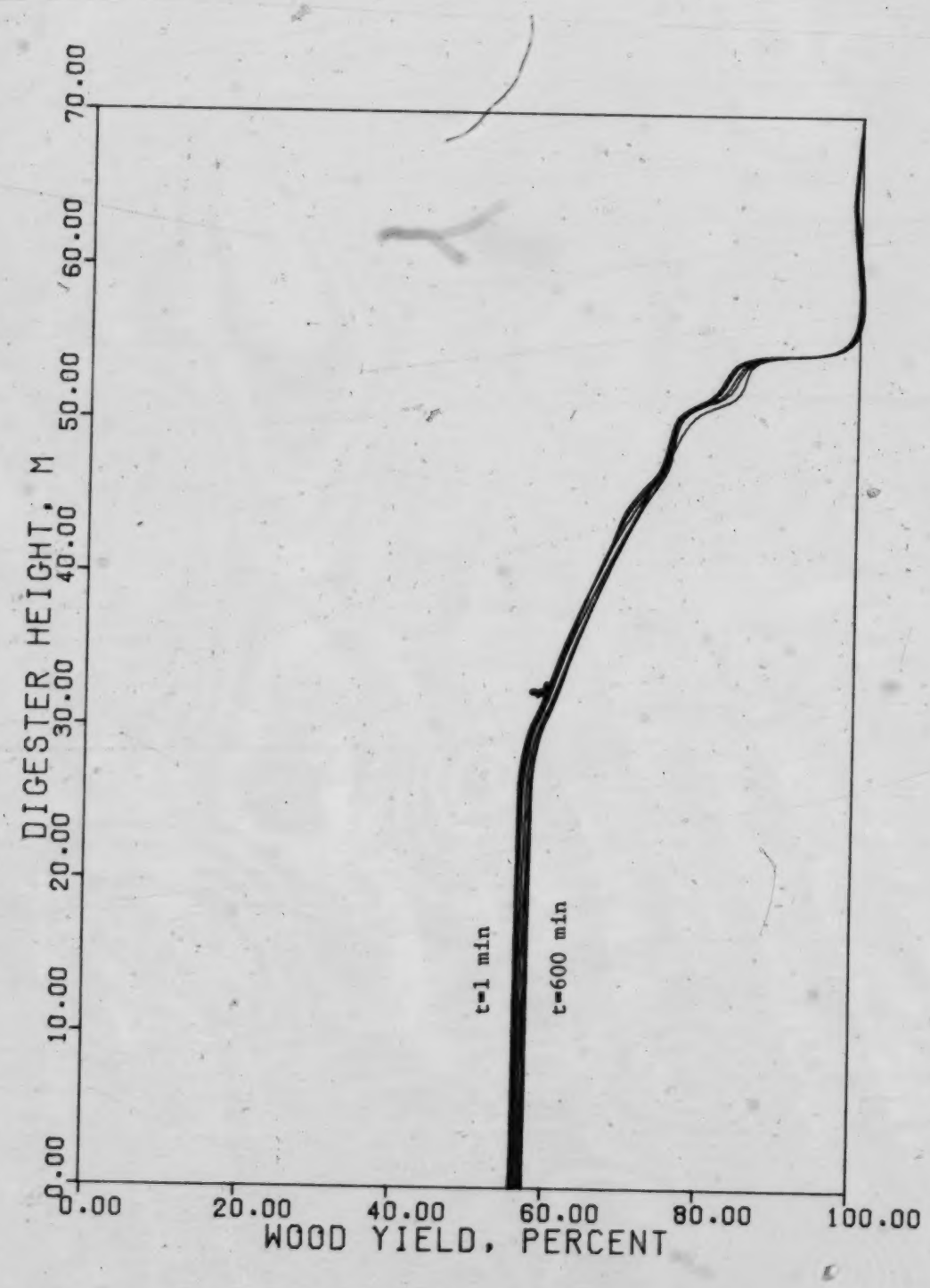


Figure 5.31 : Wood Yield Profiles for Run #8, a +10% Change in the Production Rate Relative to the Base Case (Run #1)
(The profiles are at 1, 10, 20, 50, 100, 150, 200, 250, 300, 350, 400, 450, 500, 550 and 600 minutes)

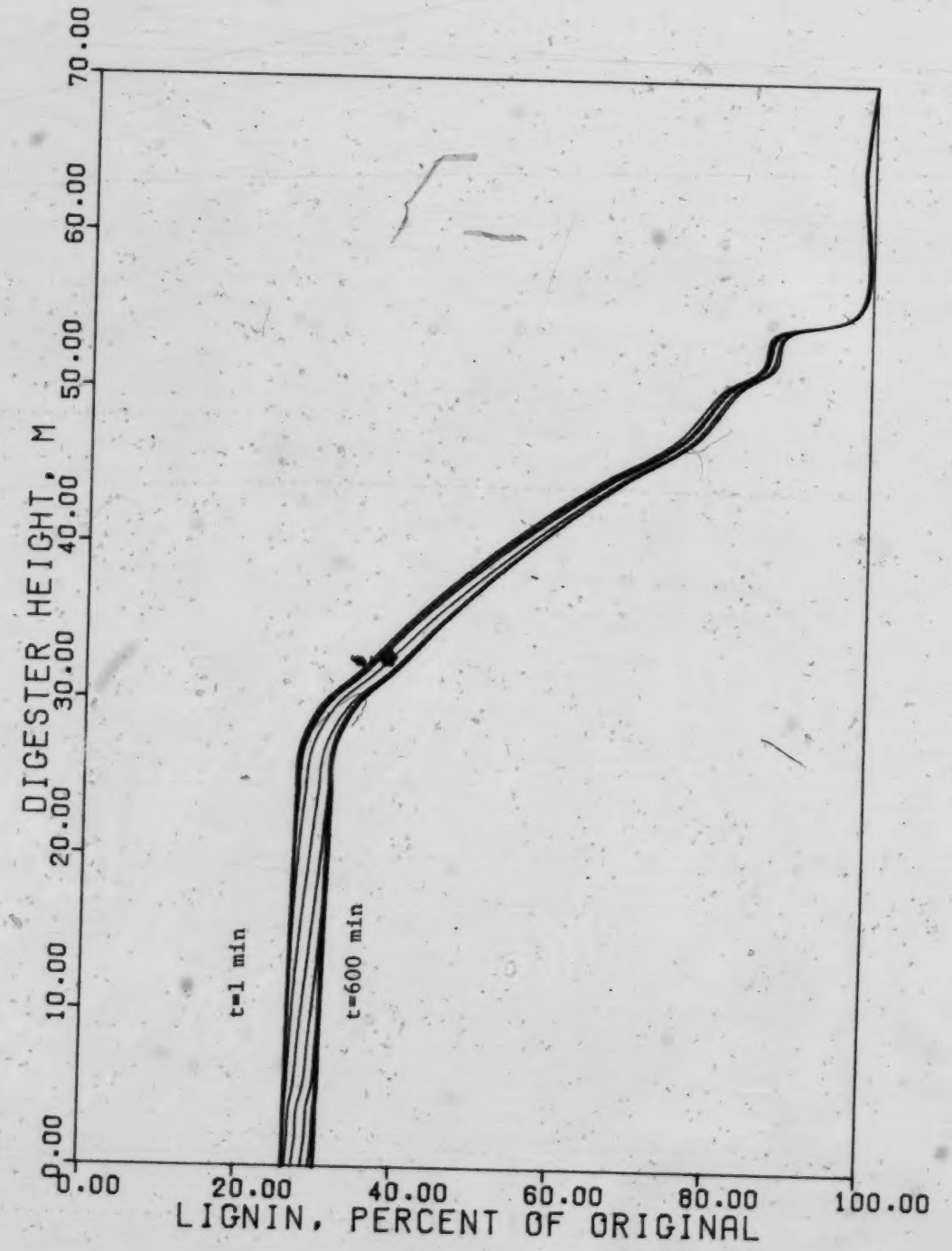


Figure 5.32 : Lignin Profiles for Run #8
(+10% Change in the Production Rate)

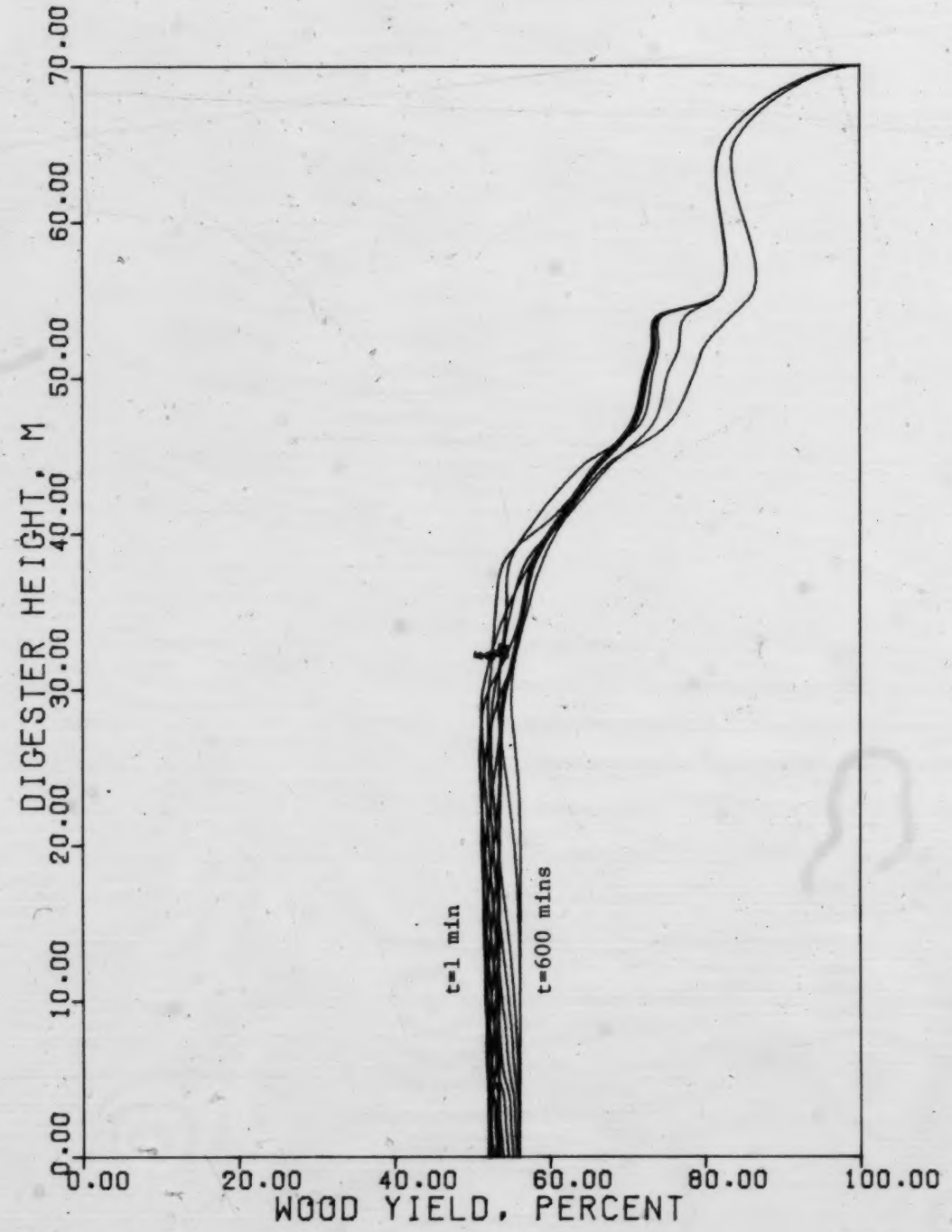


Figure 5.33 : Wood Yield Profiles for Run #9,
a Species Change from a Hardwood to Softwood
at the Base Conditions (Run #1)

The profiles are at the same times as for Run #8

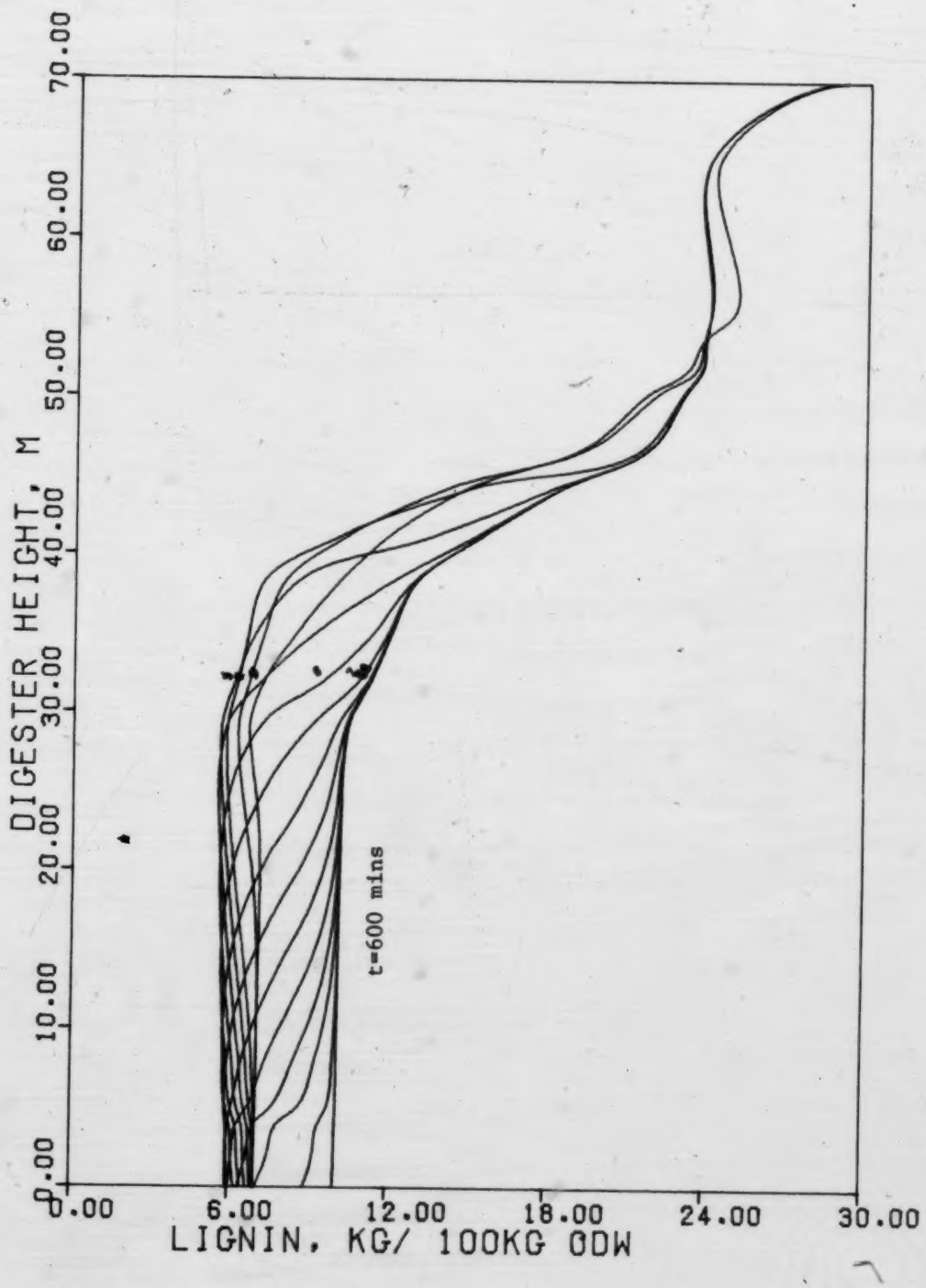


Figure 5.34 : Lignin Profiles for Run #9
(Species Change from a Hardwood to a Softwood)

5.7 Conclusions

The main operating variables used in digester control were varied and their effect on pulp yield and lignin quality analysed. As was expected, the effect of temperature was largest and, for a percentage change of the same magnitude, the effect of alkalinity is the least. The main object of these runs was to be able to show that the scalar variables that are used in the control of product quality were not always unique and this is demonstrated by the runs in sections 5.2 and 5.4. These runs also helped to show that there are a number of alternate operating conditions that could be used when operating constraints, such as would arise if a heater scaling problem was encountered. The study of cook zone length variation was possible since the model has the ability to simulate cooking in the wash zone. The cook zone length was shown to be an operating alternative although it is seldom used in industry at present.

CHAPTER SIX

CLOSED LOOP SCHEMES

This chapter includes the review of digester control schemes. First, digester control studies are examined followed by a discussion of typical digester control loops that are implemented in industry.

6.1 Review of Digester Control Schemes

The purpose of process control is simply to maximize the efficient usage of raw materials and process equipment. The digester being at the start of the pulping process has to be carefully controlled since production upsets and disturbances can carry over and affect downstream process units such as the bleach plant and the paper machines. Therefore the main objective in digester control is to maximize production by improving pulp yield and to optimize the performance of the digester so as to minimize raw material, chemical and energy costs. The other goals

are minimum variation in pulp quality as measured by Kappa Number, Permanganate Number, Chlorine Number, or fibre strength etc.; stable consistent operation of the process; changes in production rate without upsetting pulp quality; changes of pulp grade or wood chip species with minimum off-grade pulp; and optimization of the cooking chemicals recovery cycle load by better wash zone control. In recent times with computer control getting more popular, pulp mills are using computers to give improved performance. The reason for this is more consistent plant operation regardless of operating personnel capabilities.

Process control schemes and strategies in the pulp and paper industry have been reviewed by by Holm and Perry (42), Williams (104) and more recently by Perron and Ramaz (80). These articles report on the philosophy behind the design and implementation of control systems in the industry and have references to mathematical models of the processes.

Computer control was introduced to the pulp and paper industry in 1961 and the first continuous digester was brought under computer control in 1964. Both Fox (28) and Smith (90) report on the performance of the first closed

loop process computer control system for a digester. There are survey articles on the extent of digital computer usage in the industry by Brewster and Bjerring (11), Keyes (54) and Gee amd Chamberlain (32). The Brewster article was published when computer control was still in its inception in the industry and as of March 1969, there were a total of 47 computer installations in the U.S. Pulp and Paper Industry. In 1976 there were over 600 installations (54) including approximately 33 continuous digesters under computer control. This rise in the number of computer installations is due to the development of control packages by computer vendors, improvement in computer performance, decrease in hardware cost and the development of sensors which make computer control more convenient. Economic benefit from installing computers have been reported (10, 43, 98) and payout periods for such systems range between one and two years.

The problems involved in measurement, modelling and control have been described by Mayer (73) and Church (20). Measurement problems are attributed to unreliable and inaccurate sensors for wood variables like chip moisture

content, wood quality, lignin concentration and on line alkali measurement for cooking chemicals. A paper by Macleod (71) mentions that vendors are developing such instruments and that they are in the course of being throughly tested. Long time delays, measurement noise and inaccurate models in addition to sensors are blamed for most of the control problems.

Pulping models have been developed to accurately describe the cooking process and they have been discusssed in an earlier chapter. The object of such models has always been for an improved understanding of the problem with an ultimate use for better control purposes. The aim is to be able to accurately predict the output controlled variables from the process input variables. The increasing utilization of computers for control have made it imperative for better models so that a feedforward compensation type decision can be made before the disturbance significantly affects the process. One of the first studies in this regard was by Vroom (99) who derived the H-Factor. This variable is used as a combined measure of the cooking temperature and the duration of cooking and either of the

two can be adjusted for a change in the other to give a consistent degree of cooking. The work followed by Carroll (15), Kerr (52, 53), McKibbins et al (75), Service (86), Hatton (36, 37), and Boyle and Tobias (9) can be classed as statistical or mathematical models. Carroll (15) and Boyle and Tobias (9) have models for the overall pulping process while the others are limited to digester operation. These models relate the output variables like pulp yield or Kappa number to input variables such as cooking time, temperature, alkali to wood ratio and H- Factor for a particular wood species. The more detailed models include chip moisture and size and cooking liquor sulphidity. Other more detailed models by Stillman (93), Johnsson(49) and Smith and Williams (88) have been described earlier.

The increasing use of computer control has involved computer vendors in the development of various models and control packages for pulp and paper applications including continuous digester control. These packages are available on a turnkey basis and Church (20) and Gee and Chamberlain (32) have lists of vendors and their applications by process area. The Kappa Number control loop is considered the most

complex as it employs a model of the kinetics. Measurex (10, 64) use their batch digester model and a model of the pulp movement from the heating zone to the blow valve. Industrial Nucleonics (30) use an H-Factor model incorporating the lower cooking zone volume. This model assumes that the initial alkali concentration is constant (20). Foxboro (4) uses a model reference control technique with a Kappa number steady state model based on the Alkali/Wood ratio, chip temperature and the residence time and a dynamic model which includes dead time compensation on the output from the static model before the resultant predicted valve is compared with a laboratory measured Kappa number value. The error is used to adjust parameter valves in the static and dynamic models. Now some organizations are buying their own hardware and developing software "in house" to match their particular need. "Modern" control techniques have been mostly used on paper machines in the past but not for continuous digesters. Cegrell and Hedquist (18) have used linear stochastic control theory to derive a self-tuning regulator algorithm to control the Kappa number.

A survey conducted on pulping methods of 125 mills

in North America (38, 39) reported that 90% of the mills considered the cooking temperature as a valuable control variable to correct the control of a cook, 44% of them used alkali concentration and 27% used residence time in the cook zone while 25% used all three. A digester model in a three variable situation would therefore make possible an economically optimum adjustment among the variables considering pulp production and mill restraints on chemicals and energy.

The digester control system and loops are shown in the piping and instrumentation diagram, Figure 3.1 . The control system is hierarchical in design. Level zero, the lowest level, is the measurement, data acquisition, scanning, alarming and the process operators console. The next higher level one is single loop setpoint regulatory control for each of the control variables. Level two is multivariable direct control which could include cascade, ratio or feedforward. The levels one and two control loops receive their setpoints from the next higher level. Level three is supervisory control for the overall process, for production, yield, pulp quality and grade changes. The

regulatory control objectives for the three levels are chip feed rate to the top of the digester, blow flow, and chip level, chemical and liquor to wood ratios, quench and extraction temperatures, wash zone countercurrent flow control, Kappa Number and Yield. These loops are described in more detail in the following sections.

6.2 Chipmeter Control

Chipmeter rate control, Figure 6.1 regulates the chipmeter speed to maintain a constant dry wood rate to the digester. The chipmeter is dynamically calibrated each time the chip bin is emptied, as it is a volumetric device and the filling efficiency and consequently the chipmeter capacity per revolution are required. The chip moisture for an oven dry rate calculation is either calculated from a steaming vessel heat and material balance (27) which is not very accurate and large errors are not uncommon or it is read directly from an on-line sensor. These chip moisture meters will measure moisture content during summer months in Canada but are severely limited when the chips are frozen.

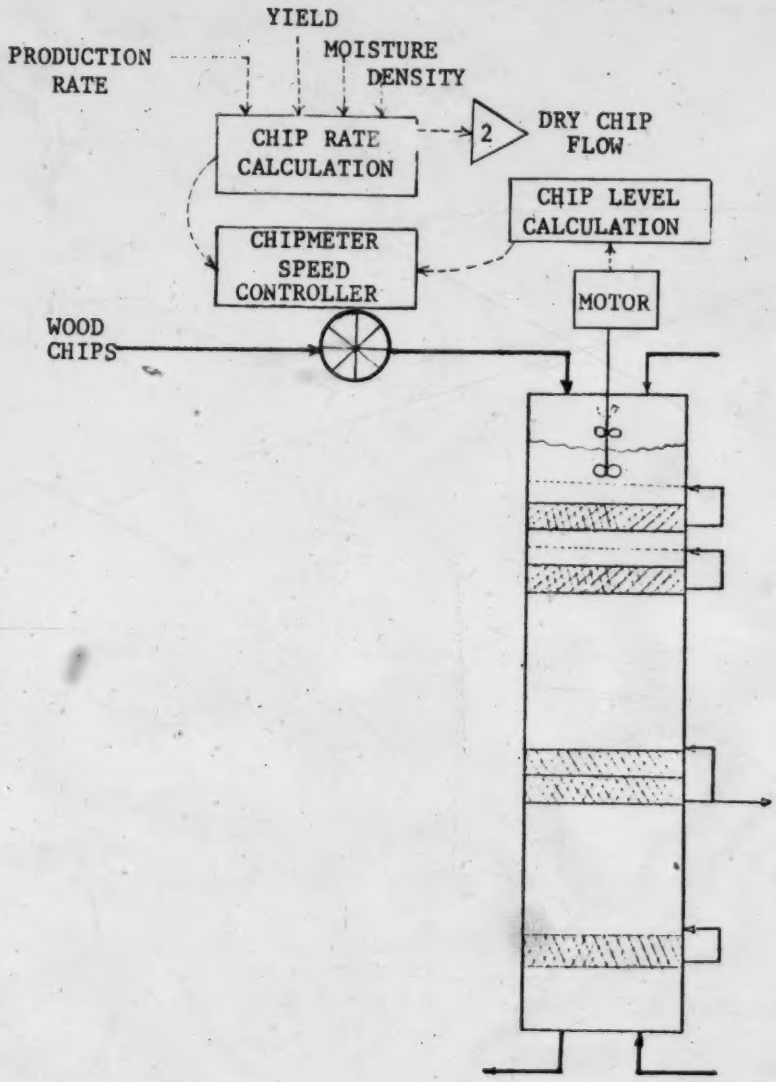


Figure 6.1 : Chip Feed Rate and Level Control

The chip packing density, moisture content and desired yield being known the computer is fed a specific production rate value and the desired chipmeter rpm is evaluated.

6.3 Chemical and Liquor to Wood Ratios Control

The flow of cooking liquor to the top of the digester is controlled to maintain the liquor to wood ratio and the alkali to wood ratio. The liquor requirements vary between mills and with the product produced. Typically, bleached papers require more liquor and chemicals. The liquor ratio could vary from 3 to 6 cubic metres of liquor/ton of dry wood and the amount of active alkali from 10 to 20 percent (kg of AA as Na2O / 100 kg of dry wood).

The chemical to wood ratio is set to keep the cooking chemicals slightly in excess of that required for delignification. The actual chemical input is calculated from white liquor concentration and flow and dry wood flow rate from the chipmeter. The white liquor flow is used as a manipulated variable to correct any imbalances. This is a sluggish control loop with a time lag of about one hour as

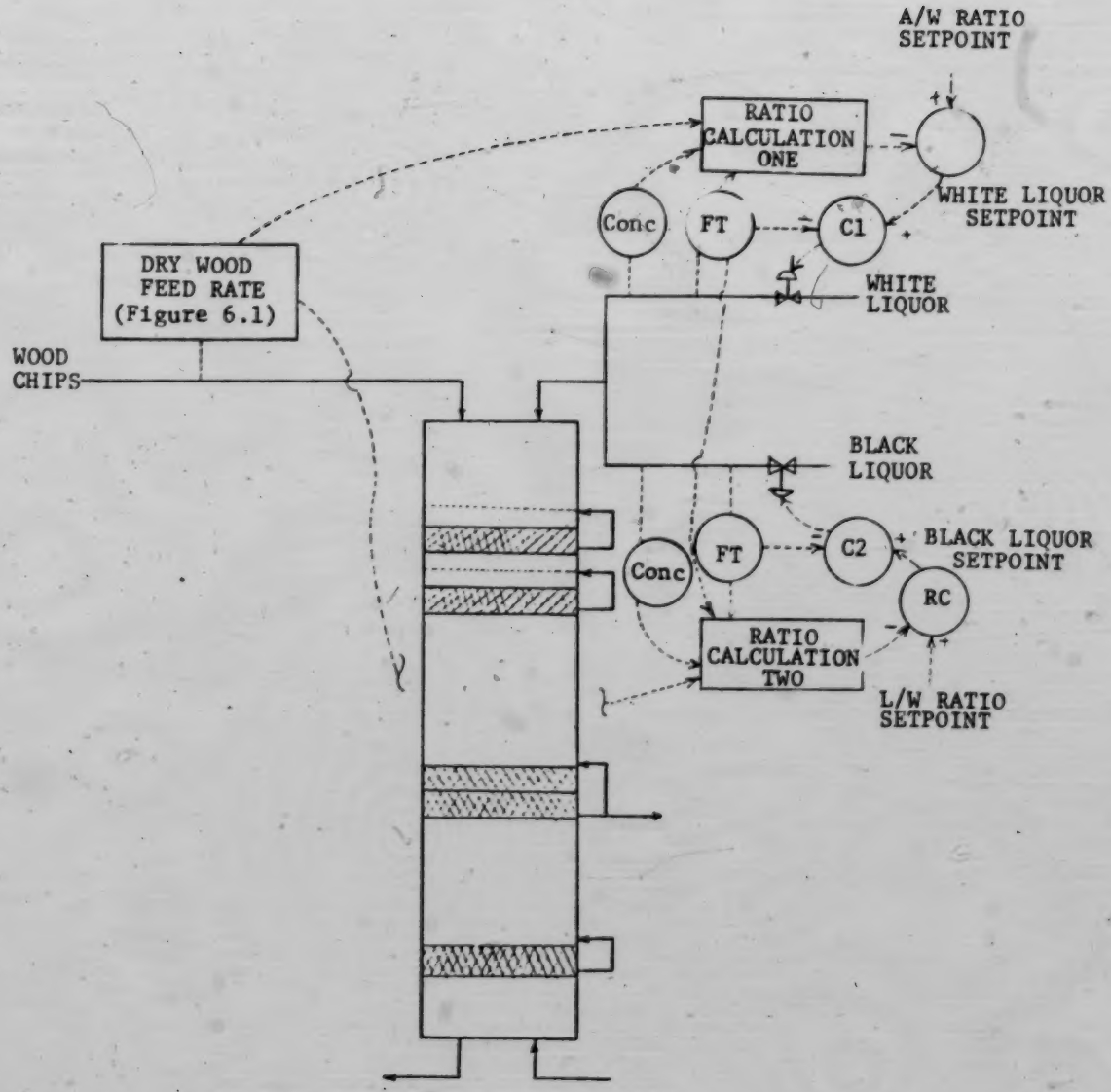


Figure 6.2 : Alkali/Wood and Liquor/Wood Ratio Control

the concentration in the top circulation rises slowly. For a rapid change the chemical concentration is allowed to overshoot the required value.

The liquor to wood ratio control is maintained by manipulating the flow of weak black liquor to the top of the digester. The liquor downflow in the impregnation and cooking zones is calculated from a volumetric flow balance about the digester. The liquor downflow originates from chip moisture, white liquor, steam condensate from the steaming vessel and the top dilution black liquor. The amount of dilution liquor added must be balanced against the heat load on the upper and lower heaters and chemical recovery load at the extraction screens. The alkali concentration is usually manually tested every hour and a reliable outline alkali sensor would be an advantage for both loops.

6.4 Chip Level Control

The chip level and blow flow are interrelated as they affect the chip residence time in the digester zones.

The chip level is evaluated from the electric current load of the stirrer in the digester top separator, Figure 6.1. The chip level controller then either adjusts the chipmeter speed and hence the chip flow at the top of the digester or the blow flow rate and consistency.

6.5 Blow Flow and Consistency Control

The blow flow and chip level are controlled to give a constant residence time in the various digester zones and primarily the cook zone (Figure 6.3). The rate of fibre discharge is dependent on the blow flow and its consistency and are set to the desired production rate. The consistency is controlled by the bottom dilution flow, digester pressure at the bottom or the bottom scraper rpm. The fibre discharge rate and the chip feed rate are in turn used in the control of chip level in the digester.

6.6 Temperature Control

Temperature of the chip mass is considered the most

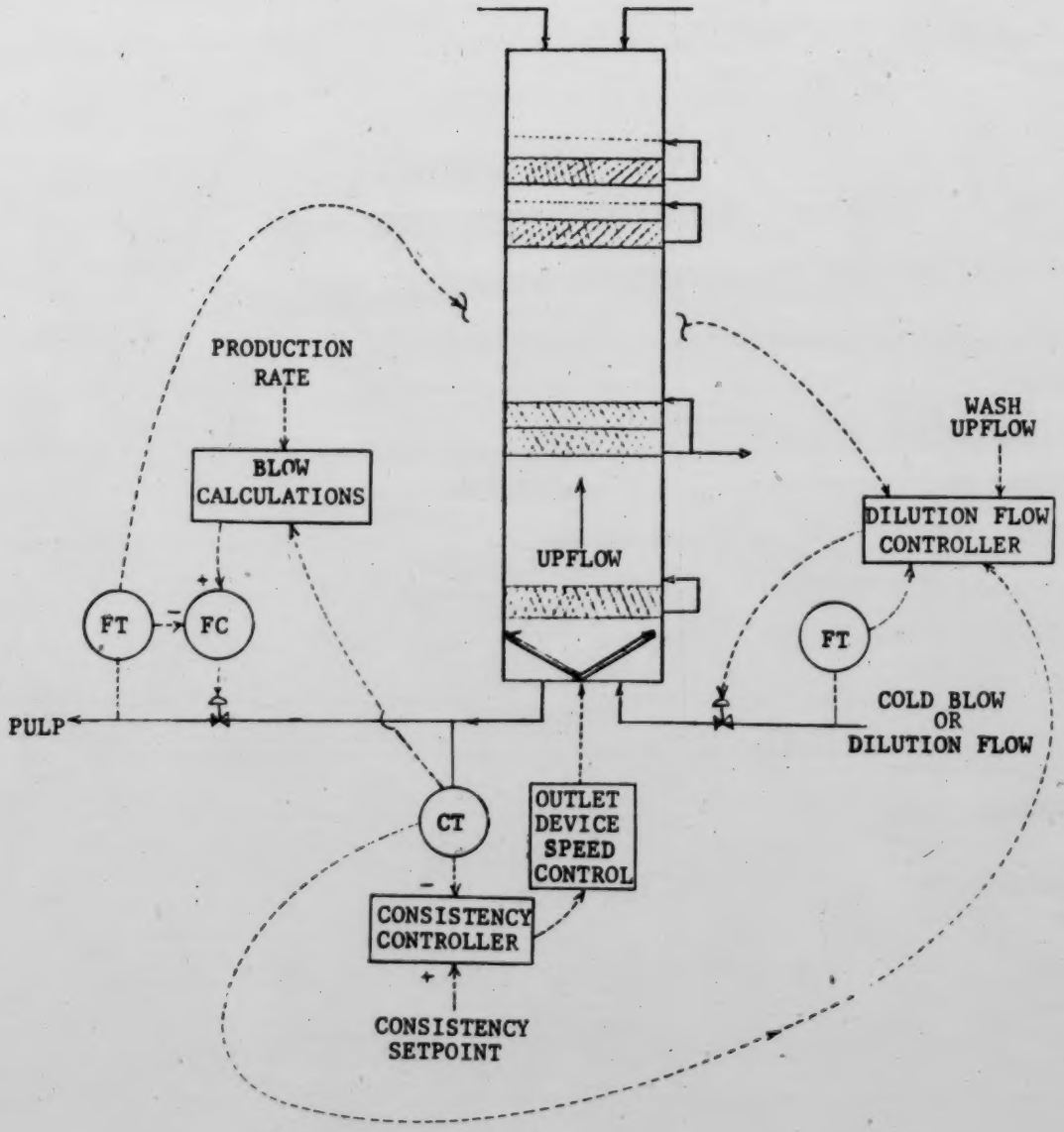


Figure 6.3 : Blow Flow and Consistency Control

important pulping variable by most mills (38), as was mentioned earlier. This is due to the large sensitivity of temperature in determining the final product quality (Kappa Number) of the pulp.

There are normally two separate heating zones in a Kamyr digester, refered to as the upper and lower heating zones. Only the controls for the lower zone are shown in Figure 6.4 as the upper zone control is similar.

The heater flows and heater entrance and exit temperatures are the only measurable variables for temperature control of chips. Since a direct temperature measurement of the pulp mass is not available, the value is estimated using a model of the heater zones. This model is just a dynamic energy balance based on the heater section. The setpoints for the two heaters are set by the Kappa number control scheme. The upper heater chip exit temperature is estimated, compared to the setpoint, and the error used as a basis for feedforward compensation in the lower heater controller. The time lag for a change in the two heater temperatures varies from five to ten minutes depending mainly on the heater flow rate entering the

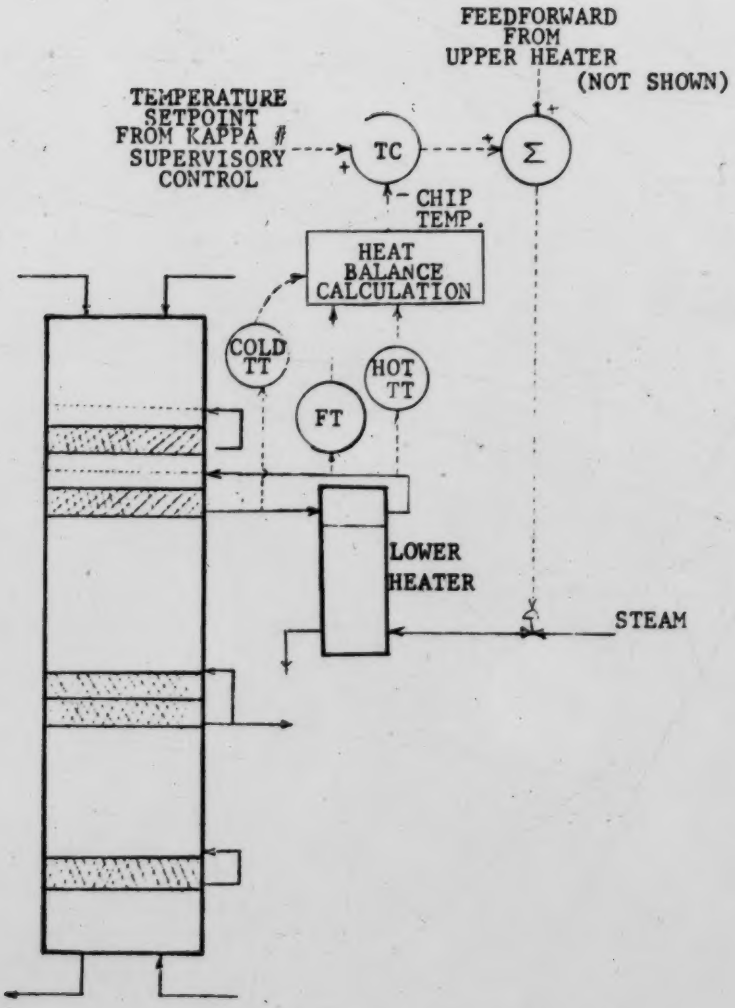


Figure 6.4 : Temperature Control

digester.

6.7 Quench and Extraction Control

After cooking is complete the spent liquor is displaced and removed at the screens before it is sent for recovery. The cooking reaction is reduced by the quench liquor just above the extraction screens as shown in Figure 6.5. The boundary between the effective cook zone and the wash zone is controlled by the extraction flow rate and the temperature of the cooler countercurrent flow of liquor from the wash zone. A cheater line from cold blow to the quench line gives independent control of the quench temperature. If the cheater line is not available then the quench temperature is dependent only on the extraction rate.

The extraction flow determines the wash liquor upflow and is manipulated to keep the wash flow at its set point. The countercurrent wash flow is estimated in one of two ways ways, a heat balance on the wash heater can be used since the heat load is proportional to the upflow or through a volumetric balance at the bottom of the digester. Wash

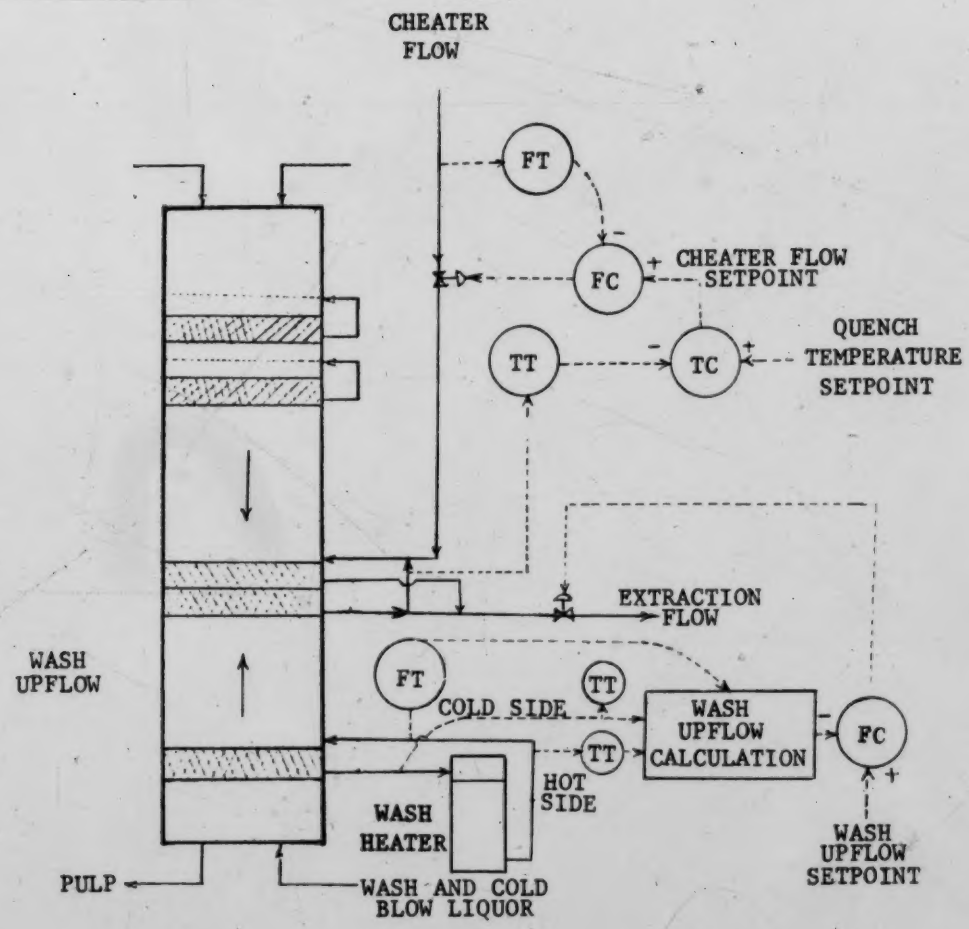


Figure 6.5 : Quench and Extraction Zone Control

flow is characterised by the dilution factor which is the ratio of wash liquor upflow to the pulp downflow in the washing zone and typical values are betweeen 2 and 3 kg of water/kg of air dry pulp. A smaller dilution factor would result in insufficient washing, i.e. reduced washing efficiency, and a larger value would put an additional burden on the wash heater and the recovery cycle. A large dilution factor would also affect the cook zone boundary at the extraction screens while a small value would extend the cook zone almost to the bottom of the digester. This is sometimes used by the operators if there is insufficient cooking in the cook zone.

6.8 Kappa Number and Pulp Yield Control

The Kappa Number and pulp yield are interrelated and equations have been developed that relate the two variables for a particular wood species, e.g. Johnsson (49), Rydholm (81 p635) and Smith and Williams (88). Therefore, in most cases the pulp yield versus the lignin concentration relationship is known by mills for the wood

species that they process. The Kappa number, and hence the yield, is usually regulated by the upper and lower heater outlet temperatures. Since the Kappa number is the most important variable for determining final pulp quality precise temperature control is vital. The H-Factor which combines both the cooking time and temperature is also used as a measure of the degree of cooking. The aim is to cook the wood chips to a lignin content in its bulk reaction rate phase instead of the residual reaction phase where the rate of cellulose removal is faster than that of lignin. The temperature and the residence time in the cook zone are the only two variables that would affect the pulp quality once the chips are in the cook zone. The cook zone residence time is only adjusted when a change in production rate is desired, if there is a restraint on steam flow and a higher cook temperature is desired, or when the chips are not sufficiently cooked and the operator would like the cooking to proceed into the wash zone.

A steady state model of the digester is used to calculate the Kappa Number based on the Alkali/Wood ratio, the cooking temperature and the residence time in the cook

zone as shown in Figure 6.6. One of the three operating variables is adjusted based on the current operating constraints. The pulp yield or the Kappa Number from the blow line is analysed typically every hour and the error fed back to correct for drift in the model parameters. The model is used to compensate for the long time delay between the end of the cook zone and the time, a sample is analysed before the lower heater temperature is adjusted.

6.9 Production and Grade Change Control

Production rate and grade changes can be made in a scheduled or unscheduled manner and both have different operating procedures. The planned changes can be due to production demand, a different grade requirement or introduction of a different wood species. An unscheduled change is usually due to a bottleneck in the chipyard or chip bin or to meet sudden upstream or downstream demands for a change in production rate. The goal in both cases is to make the switch as smooth as possible with minimum disturbance towards quality and yield.

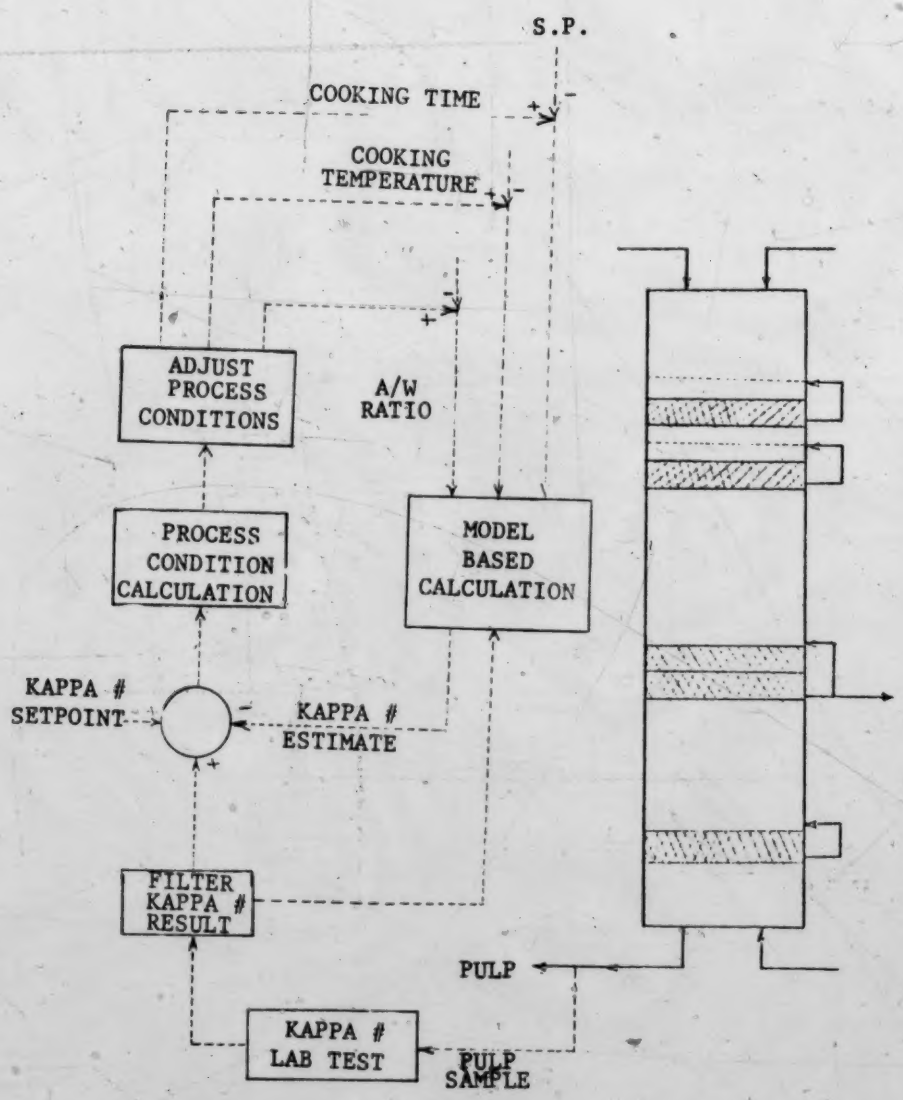


Figure 6.6 : Kappa Number Control

For scheduled changes the heater temperature is gradually changed and the chemicals suddenly changed to a new value that is followed by a gradual change in the production rate. For an emergency change the chip feed rate, heating zone temperatures and liquor flows are rapidly changed to new setpoint values. This is to minimize the pulp quality and yield transients which cannot otherwise be avoided. A grade change is similar to a production change and is treated similarly. This change can be due to a yield or Kappa number change with the same species. A change of wood species results in changes in bulk density, cooking rate and yield. The object is to produce pulp which has the desired properties when the new species arrives at the blow line without producing a hard or soft pulp during the interim period. This is achieved by changing the operating parameters as the species interface moves through various digester zones. The parameters that are changed are the liquor to wood and chemical to wood ratios, cooking temperature and the wash target. An unscheduled species change requires rapid computation of new conditions but they are implemented in an identical manner.

CHAPTER SEVEN

CONCLUSIONS AND FUTURE WORK

The conclusions and recommendations for further work are presented.

7.1 Conclusions

A nonlinear, dynamic model of a continuous Kamyr digester has been developed and used in open loop simulation studies. Since industrial digesters do not normally have an extensive number of sampling ports or sensors, it has not been possible to obtain the data necessary for a direct comparison of concentration profiles and/or time histories. However, individual modules of the program have been tested separately and the total program produces results that are intuitively correct and which compare favourably with the results of previous studies.

Some compromises and approximations were made, especially in the area of chemical kinetics to keep the overall program size and execution time to a reasonable

level but the program is very general in terms of what configurations, operating conditions and disturbances it will handle. All the digester dimensions, physical properties, physical properties etc. can be set by modifying input data, or in some cases portions of specific subroutines. Operating conditions can be set by the user and are specifically programmed to facilitate closed loop control studies. The program will simulate the dynamic response to chip moisture disturbances, species changes, changes in inlet liquor flow and/or concentration, plus changes in heater circulation flows and/or temperatures. The model includes thirteen state variables in the dynamic equations, allows for all cooking reactions to proceed into the wash zone, and includes optional features such as the use of 'cheater' flow for the independent adjustment of quench temperature.

Separate versions of the program are also available to simulate batch digesters and to produce steady state profiles and histories. These programs were used to produce an 'independent' check on results.

The results of the general simulation program are available in three forms. First, as profiles of any of the

state or derived variables such as lignin concentrations, temperature, Kappa number etc. plotted versus digester height. These plots define the operation of the digester at any instant of time. Second, the program can produce 'history plots' of operating conditions or variables, such as lignin concentration versus time. These plots define the operating conditions used and the state variables which characterizes the pulp from the time a particular unit of pulp enters the digester until it leaves the blow line. Third, the program produces listing of the steady state profiles plus summaries of the operating conditions and configuration. One of the recommendations arising from this work is that industry consider generating the profiles on-line and use them for operator guidance or process control. This should permit significant improvements in product quality and uniformity because at the present time the exit pulp quality cannot be measured directly by any on-line set of measurements nor can the inlet digester conditions required to produce a pulp of specified quality be easily determined. Presently, the operators use scalar measures of pulp quality such as H-Factor, residual lignin concentration, Kappa number etc. for control purposes.

However, as shown by simulation results from this study (and as is undoubtly found in industrial practice) the same scalar measures, such as Kappa number at the blow line, can be produced using significantly different operating conditions. It is almost certain that the actual production history of a particular unit of pulp would influence its downstream processing characteristics such as 'bleachability' and/or final product specifications such as paper strength, smoothness etc. The display of instantaneous digester profiles should make it possible for the digester operator to control the digester operation more closely and to improve reproducibility. Use of displays showing the production history of the unit of pulp currently entering a downstream process, such as the bleach plant, should improve control and product quality in these downstream units.

Use of a simulation program such as the one developed in this work, in parallel with actual digester operation would permit the process operators to evaluate alternatives for implementing chip species changes, grade changes and/or production rate changes. Displays of instantaneous profiles and historical plots would show the

progress of changes through the digester and hence provide a basis for operator control to improve response times and reduce off grade pulp. Careful tuning of the parameters of the dynamic model would be required but simulation of startup dynamics (c.f. Figures 5.1-5.5) and optimization studies to reduce energy consumption or balance tradeoffs between chemical consumption and pulp quality are also possible (c.f. Chapter 5, where the effects of changes in cooking temperature and chemical concentration were demonstrated). The parameters in the dynamic model such as reaction rate constants, diffusion coefficients, heat transfer coefficients, pulp density etc. plus their dependence on operating conditions such as temperature, should obviously be 'tuned' via a continuing project involving production and development personnel.

7.2 Future Work

As suggested above the dynamic model developed as a part of this project has significant potential for effective industrial utilisation. However, one of the prime motivations in developing this model was to provide a

convenient and efficient means of evaluating improved computer control techniques - especially at the higher or supervisory levels. Some specific approaches that appear to have significant potential for industrial use include :

i) Material and energy balance control schemes to coordinate the supervision of individual DDC loops.

ii) On-line constraint identification, using techniques such as linear programming followed by appropriate modification of operating conditions and/or objectives.

iii) Use of modern multivariable control techniques such as those investigated previously in this department (26). [1]

For example :

a) time delay compensation (38-A),

b) frequency domain designs to 'decouple', i.e. reduce interactions between controlled variables (62),

[1] the following references are to the individual theses. Several papers based on these projects were published subsequently in different journals.

c) use of filters and/or observers to estimate variables that cannot be measured directly (33, 79),

d) control of closed loop system response and/or parameter sensitivity by eigenvalue and eigenvector assignment (87),

e) 'optimal' manipulation of input variables to achieve minimal time response in the presence of operating constraints (77).

iv) Self tuning regulators (19, 82), and hyperstable adaptive control systems that require only input/output measurements for the plant (50).

v) Supervisory and distributed system control concepts that would permit feedforward, feedback and adaption of information among all the major units in a mill from the digester to the paper machine. For example, factors such as the bleachability of the pulp and the quality of paper produced from it, provide the ultimate means of evaluating digester operations and globally optimize economic behaviour. A computer system is required for such feedback and evaluation.

vi) The kinetic model used in this study is too simple to accurately represent the complex set of pulping reactions. Present research includes development of processes to reduce hemicellulose degradation by addition of chemicals such as anthraquinone in the cooking liquor. Studies have also been done for reprecipitation of the carbohydrates during the later portion of the cook. Accurate simulation models for such processes are required. Cooking data for various wood species which would assist in parameter estimation for these models is also needed.

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APPENDIX A

DERIVATION OF MODEL EQUATIONS

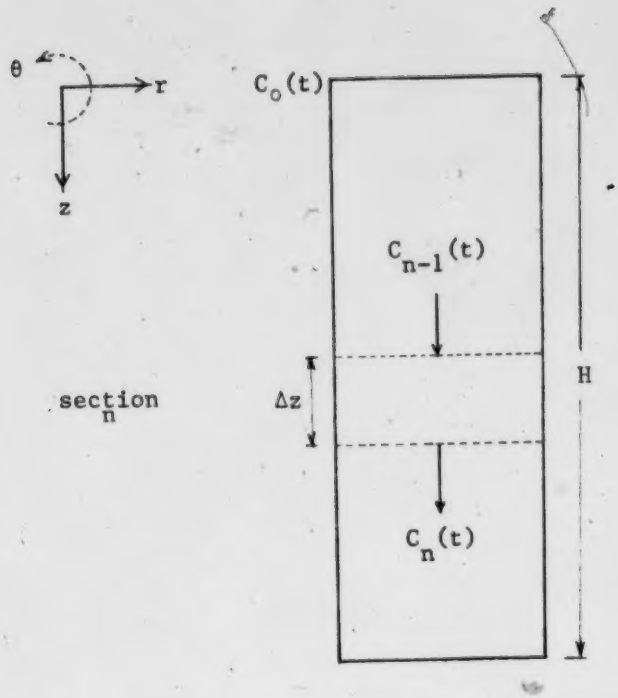
This appendix is in support of material covered in chapter three. The partial differential equation is derived first and the set of thirteen nonlinear ordinary differential equations in the next section.

A.1 Partial Differential Equation

The unsteady state wood component mass balance was derived in cylindrical coordinates. The equation can also be found in a standard textbook (eg. Bird, Stewart and Lightfoot, 6, p559, Table 18.2-2 Eqn B) :

$$\frac{\partial C}{\partial t} + \left\{ v_r \frac{\partial C}{\partial r} + \frac{v_\theta}{r} \frac{\partial C}{\partial \theta} + v_z \frac{\partial C}{\partial z} \right\} = D \left\{ \frac{1}{r} \frac{\partial}{\partial r}\left(r \frac{\partial C}{\partial r}\right) + \frac{1}{r^2} \frac{\partial^2 C}{\partial \theta^2} + \frac{\partial^2 C}{\partial z^2} \right\} + R \qquad \text{(A.1-1)}$$

where C is a wood component concentration, v_r, v_θ, and v_z are the velocity components in the three directions, r is the radius, D is the diffusion coefficient and R the total reaction term i.e. the rate of production per unit volume.; (The nomenclature is summarized in a table at the end of this appendix.)



Neglecting the radial (r), angular (θ)components and the diffusion coefficient, D. Equation (A.1-1) reduces to :

$$\frac{\partial C}{\partial t} + v_z \frac{\partial C}{\partial z} - R = 0 \qquad \text{(A.1-2)}$$

The same equation can be written in functional terms as:

$$\frac{\partial C(z,t)}{\partial t} + v_z(z) \frac{\partial C(z,t)}{\partial z} - R(C,z,t) = 0 \qquad \text{(A.1-3)}$$

The boundary conditions for this case are :

$$C(0,t) = C_o(t) \quad \text{at } z=0 \text{ and } t \geq 0 \qquad \text{(A.1-4)}$$

$$C(z,0) = C(z) \quad \text{at } t=0 \text{ and } 0 \leq z \leq H \qquad \text{(A.1-5)}$$

Discretizing equation (A.1-2) around z

$$\frac{dC_n(t)}{dt} + v_{z,n} \frac{\Delta C_n(t)}{\Delta z} - R_n(C_n,t) = 0 \qquad \text{(A.1-6)}$$

or when multiplying throughout by the volume of section n in the digester, V_n

$$V_n \frac{dC_n(t)}{dt} + V_n v_{z,n} \frac{C_{n-1}(t) - C_n(t)}{\Delta z} - V_n R_n(C_n,t) = 0$$

or, assuming constant crossectional area in each section

$$V_n \frac{dC_n(t)}{dt} + Q_n(t) \{C_{n-1}(t) - C_n(t)\} - V_n R_n(C_n,t) = 0 \qquad \text{(A.1-7)}$$

The boundary conditions (A.1-4) and (A.1.5) reduce to :

$$C(0,t) = C_o(t) \text{ at } z=0 \qquad \text{(A.1-8)}$$

and

$$C(z_n,0) = C_{n,o} \text{ at } t=0 \qquad \text{(A.1-9)}$$

respectively, where C_o is the concentration value entering at the top of the digester and $C_{n,o}$ is the initial, starting concentration in section n, and Q_n is volumetric flow rate, i.e., $Q=V_n v_{z,n}/\Delta z$.

The same equations if derived for the chemical components in the free and entrapped cooking liquor would have an additional diffusion term for mass transfer between these two phases.

A.2 Ordinary Differential Equations

The set of nonlinear ordinary differential equations are presented here for a digester section n :

Overall mass balance :

$$V_n \frac{d\rho_n}{dt} = V_n \, \text{Func}(z_{n-1}, z_n, \text{HFAC}, t) \qquad \text{(A.2-1)}$$

where

V_n is volume of section, m^3

ρ_n is the density (compaction), kg/m^3

z_{n-1}, z_n is position of section n, m

HFAC is the H-Factor and a measure of degree of cooking

Individual wood component balances :

The individual wood component balance in terms of X_n, the wood specie concentration in section n is :

$$\rho_n V_n \frac{dX_n}{dt} = w_{n-1} X_{n-1} - w_n X_n - R_{x,n} \qquad \text{(A.2-2)}$$

where

w_n is the wood flow rate from n in kg ODW/min

and $R_{x,n}$ is the total reaction term, hydroxide & sulphide

i.e. $$R_{x,n} = (k_i C_{el,OH,n} + k_{i+1} C_{el,S,n}) X_n \qquad \text{(A.2-3)}$$

where

k_i is the hydroxide kinetic constant and is a function of temperature, chemicals and wood component concentrations,

k_{i+1} is the sulphide kinetic constant and is related in a similar manner as k_i,

$C_{el,OH,n}$ is the entrapped liquor hydroxide concentration in section n,

and $C_{el,S,n}$ is the sulphide concentration in the entrapped liquor.

Entrapped liquor component balances :

The material balance for liquor component Y in the entrapped liquor is :

$$V_{el,n} \frac{dC_{el,y,n}}{dt} = Q_{el,n-1} C_{el,y,n-1} - Q_{el,n} C_{el,y,n} + k_m a \left(C_{fl,y,n} - C_{el,y,n} \right) - \left(\alpha_1 R_{l,y,n} + \alpha_2 R_{c,y,n} + \alpha_3 R_{m,y,n} + \alpha_4 R_{x,y,n} \right) \quad \text{(A.2-4)}$$

where the first two terms are convection flow terms with $Q_{el,n}$ being the entrapped liquor flow rate from section n, $C_{el,y,n}$ is the entrapped liquor concentration for the component y in the section. The α's are the stoichiometric coefficients for the four wood components and liquor chemicals and are used to calculate the chemical usage while the R's are the reaction terms (e.g. $R_{l,y,n}$ is the rate of reaction of lignin with chemical y in section n).

Free liquor component balances :

The free liquor balances for hydroxide, sulphide and reaction products are represented by the general component equation :

$$V_{fl,n} \frac{dC_{fl,y,n}}{dt} = Q_{fl,n-1}C_{fl,y,n-1} - Q_{fl,n}C_{fl,y,n} - k_m a\,(C_{fl,y,n} - C_{el,y,n}) \qquad (A.2\text{-}5)$$

these terms are similar to those in the entrapped liquor equation (A.2-4) with a convection and mass transfer term. The $k_m a$ term is the overall mass transfer coefficient times area at the section temperature.

Energy balances :

The energy balance equations for wood and entrapped liquor; and free liquor follow :

$$m_{t,wel,n}\,\bar{C}_p \frac{dT_n}{dt} = (w_{n-1}C_{p,w}T_{n-1} - w_n C_{p,w}T_n) + (w_{el,n-1}C_{p,l}T_{n-1} - w_{el,n}C_{p,l}T_n) + \Sigma R_i \Delta R_i + ha\,(T_{f,n} - T_n) \qquad (A.2\text{-}6)$$

in this equation

$C_{p,w}$ and $C_{p,l}$ are specific heats of wood and liquor respectively and $\bar{C}_p$ is the average for the two,

$w_{el,n}$ is the entrapped liquor mass flow rate,

ΔR_i is the heat of reaction for wood component i,

R_i is the reaction term,

and ha is the heat transfer coefficient times area between the wood and free liquor.

The free liquor energy balance is :

$$w_{fl,n}\, C_{p,l}\, \frac{dT_{f,n}}{dt} = (w_{fl,n-1} C_{p,l} T_{f,n-1} - w_{fl,n} C_{p,l} T_{f,n}) - ha\,(T_{f,n} - T_n) + H_{wall} \qquad (A.2\text{-}7)$$

the free liquor equation has similar terms to the earlier equation (A.2-6) except for the heat conduction from the walls term, H_{wall}.

A.3 Nomenclature

Specific

a	interfacial area between wood and free liquor
C	concentration of wood component
C_o	concentration of wood component at the top of the digester
$C_{n,o}$	wood concentration in section n at time zero
$C_{el,y,n}$	concentration of component y in entrapped liquor
$C_{fl,y,n}$	concentration of component y in free liquor
C_{pl}	specific heat of liquor
C_{pw}	specific heat of wood chips
$\overline{C}_p$	average specific heat of wood and entrapped liquor
D	diffusion coefficient
h	overall heat transfer coefficient
H	total height of digester
H_{wall}	heat transfer through walls of digester
HFAC	H-Factor, a measure of cooking history
k_i	reaction rate constant for hydroxide
k_{i+1}	reaction rate constant for sulphide
k_m	overall mass transfer coefficient
$m_{t,wel}$	total mass of wood and entrapped liquor in section
Q	volumetric flow rate
Q_{el}	volumetric flow rate of entrapped liquor
Q_{fl}	volumetric flow rate of free liquor
r	radius of section, radial component in cylindrical coordinates
R, R_i	total reaction term for wood component
$R_{x,n}$	total reaction term for wood component x in n
R_i	heat of reaction

Specific

t	time variable
T	wood and entrapped liquor temperature
T_f	free liquor temperature
v	velocity component
V	volume of section
V_{el}	volume of entrapped liquor in section
V_{fl}	volume of free liquor in section
w	wood mass flow rate
w_{el}	mass flow rate of entrapped liquor
w_{fl}	mass flow rate of free liquor
X	concentration of wood component x
z	position vector, axial distance, cylindrical coordinates

Greek Letters

$\alpha_1,..,\alpha_4$	stoichiometric coefficients for wood components and entrapped liquor chemicals
ρ	density of wood chips
θ	angular component in cylindrical coordinates

Subscripts

el	entrapped liquor variable
fl	free liquor variable
n	variable from section n
r	radial component in cylindrical coordinates
θ	angular component in cylindrical coordinates
z	axial component in cylindrical coordinates

APPENDIX B

MODEL TESTING RESULTS

This appendix is related to the description of the model that was presented in Chapter Four. Results from testing of integration routines are presented in the first section and testing of the open loop model and the kinetic model in the other two.

B.1 Testing of Integration Routines

The four integration routines tested for subsequent use in the digester model were variations of the fourth order Runge Kutta type and a predictor corrector method. The simple Runge Kutta routine was programmed in Fortran while the other three were taken from two subroutine packages (39, 72). The routines Runge Kutta Gill (RKGS) and Hamming's Predictor Corrector (HPCG) were taken from the IBM Scientific Subrcutine Package (SSP) and the Runge Kutta Merson (DASCRU) from the IMSL package. The routines were used to integrate the equations ten times sc that a

reasonable values for CPU time could be obtained.

The first set of equations used in testing the routines were linear and the analytical solution of which was in exponentials .

The equation set was :

$$\frac{dY(1)}{dt} = -\frac{1.0}{Y(2)}$$

$$\frac{dY(2)}{dt} = \frac{1.0}{Y(1)} \qquad \text{(B.1.1)}$$

and the conditions at time zero were Y(1) = Y(2) = 1.0. The analytical solution for this problem is :

$$Y(1) = \exp(-t)$$

$$\text{and } Y(2) = \exp(+t) \qquad \text{(B.1.2)}$$

Table B.1 shows the computing time used in CPU seconds on an Amdahl 470/V6 computer and the solutions obtained from the integration routines.

The second set used was a slightly stiff set of equations, and they are as follows:

$$\frac{dY}{dt}(1) = -0.1*Y(1) - 49.9*Y(2)$$

$$\frac{dY}{dt}(2) = -50.0*Y(2)$$

$$\frac{dY}{dt}(3) = 70.0*Y(2) - 120.0*Y(3) \qquad \text{(B.1.2)}$$

The initial conditions in this case were, Y(1) = Y(3) = 2.0 and Y(2) = 1.0. This equation can be solved analytically also and the integration results for this test are given in Table B.2. Based on these two tests the Runge Kutta Gill and Predictor Corrector routines were definitely inferior to the simple Runge Kutta and Runge Kutta Merson methods based on accuracy and computing time usage.

The third test was on the digester model equations where the final solution was known. This was one of the trivial tests with no reaction and also no heat and mass transfer between the wood and liquor. The Runge Kutta Gill and Predictor Corrector routines were not tested for this case. Two profiles were calculated and results from both methods were identical. The CPU time for the Runge Kutta was 1.750 seconds and that for the Merson method 3.235 seconds. This showed that the simple Runge Kutta routine was performing much better than the other routines when the problem was simple and the nonlinearities not very severe. The actual digester equations are extremely nonlinear especially in the vicinity of the heater sections where the pulp temperature is raised by at least thirty degrees

Celsius. The Runge Kutta routine was not able to outperform the Merson routine in this case and very small step sizes had to be used to obtain reasonable results. The Merson routine was for this very reason used to solve the nonlinear equations in the batch and continuous digester models.

Table B.1 Integration Table for Equation Set 1

INTEGRATION METHOD	Y at time 5	CPU sec	Y at time 10	CPU sec	Y at time 15	CPU sec	Y at time 20	CPU sec
Runge Kutta step size of 0.10	0.148417E+03 0.673766E-02	0.173	0.220294E+05 0.453923E-04	0.224	0.327009E+07 0.305787E-06	0.254	0.485454E+09 0.205979E-08	0.293
Runge Kutta Merson	0.148426E+03 0.673726E-02	0.216	0.220323E+05 0.453867E-04	0.324	0.327006E+07 0.305735E-06	0.380	0.486008E+09 0.205746E-08	0.540
Runge Kutta Gill	0.148444E+03 0.673614E-02	0.243	0.220427E+05 0.453607E-04	0.322	- -	0.555	- -	0.587
Hamming's Predictor Corrector	0.148431E+03 0.673671E-02	0.204	- -	0.267	- -	0.275	- -	0.275
Actual Values	0.148413E+03 0.673795E-02		0.220265E+05 0.454000E-06		0.326902E+09 0.305902E-08		0.485165E+09 0.206115E-08	

Table B.2 Integration Table for Equation Set 2

INTEGRATION METHOD	Y at time 1.0	CPU sec	Y at time 2.0	CPU sec
Runge Kutta with step size of 0.01	0.904830E+00 0.200645E-21 0.200645E-21	0.227	0.818722E+00 0.402587E-43 0.402587E-43	0.323
Runge Kutta Merson	0.904827E+00 0.579213E-14 0.137759E-06	0.275	0.818719E+00 -0.319808E-27 0.673490E-06	0.356
Runge Kutta Gill	0.904811E+00 0.200469E-21 0.200469E-21	0.363	0.818680E+00 0.397016E-43 0.397016E-43	0.563
Hamming's Predictor Corrector	0.904353E+00 0.101254E-21 0.143771E-02	0.342	0.818675E+00 0.348709E-43 0.354885E-03	0.529
Actual Values	0.904840E+00 0.192870E-21 0.192870E-21		0.818730E+00 0.372010E-43 0.372010E-43	

B.2 Open Loop Model Testing

The program subroutines were tested in parts and the test and results were as follows :

Table B.3 Open Loop Program Testing

PROGRAM SEGMENT	TEST	RESULT
Digester Configuration Calculation	Volumes and Areas calculated manually	Results agreed perfectly
Evaluate liquor density & its variation with temperature	Density values calculated at different temperatures	Values were within 0.1% of those in the International Critical Tables
Sodium Sulphide hydrolysis routine	Varying NaOH & Na2S Concentrations and Temperature	Results checked with Martin's (64) data. Errors were large (Max 12%) at low temperatures & high sulphidities

.... continued

Table B.3 continued

PROGRAM SEGMENT	TEST	RESULT
Sodium Sulphide available to degrade carbohydrates	Print out of values at different process conditions	Subroutine worked well. Part of the batch model
Residual reaction phase breakpoint	Check subroutine working	" "
Reaction velocity constants	Kinetic constants at various process conditions	Values agreed fairly well with Stillman (81) data
Mass transfer Coefficient calculations	Checks at various temperatures	Data from Smith & Williams (76).
Perfect mixing calculations for external flows	Hand calculations for material and energy balances	Calculations match
Calculation of Compaction values as a function of position & history	Values for position down the digester & with various cooking histories	Agree well with Hamilton's (29) data
Digester entering conditions at the top	Check working with hand calculations	Results match

.... continued

Table B.3 continued

PROGRAM SEGMENT	TEST	RESULT
Differential Equation subroutine Runge Kutta Merson method for solution of equation set Routines for solving cocurrent & counter-current flow problem Mainline, driver program	Test on sample equations and for trivial tests. i.e. no reaction & mass transfer, no heat transfer	Results are as expected. i.e. constant wood component profiles & entrapped liquor concentrations

B.3 Kinetic Model Testing - Batch Model Working

The Kinetic Model that was described in Chapter Three was tested by using a batch digester model that was written specifically for that purpose. The batch model had the same type of thirteen nonlinear differential equations as in the continuous model except that the flow terms were deleted. The results from this model were tested against cooking data collected by Daleski (19) and Smith and Williams (88) and the kinetic parameters were tuned accordingly to give the best possible fit. The computer model is such that if better kinetic data for a particular species were available it could be read in and used for simulations. The constants given in Table 2 are average values for hardwood and softwood species and were used to generate the plots that are shown in Figures B.1 to B.5.

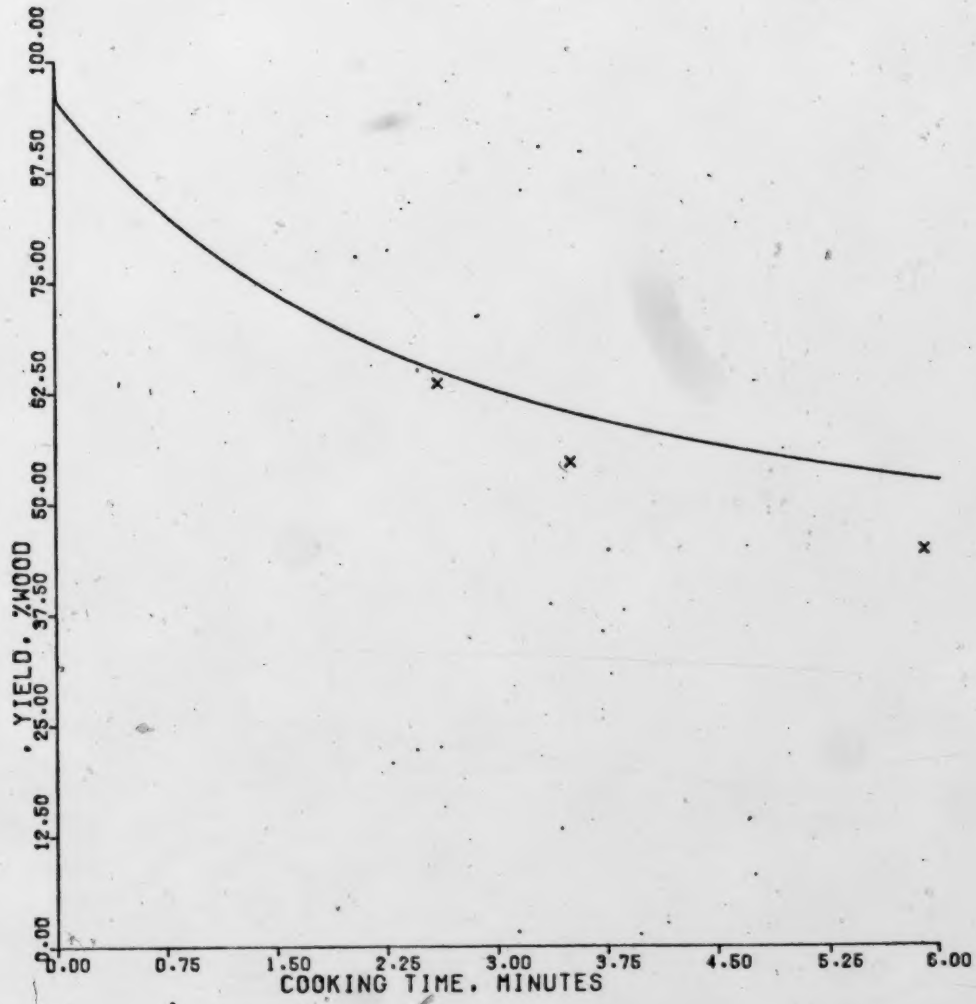


Figure B.1 : Batch Cook, Yield at 195 °C (Daleski (19))

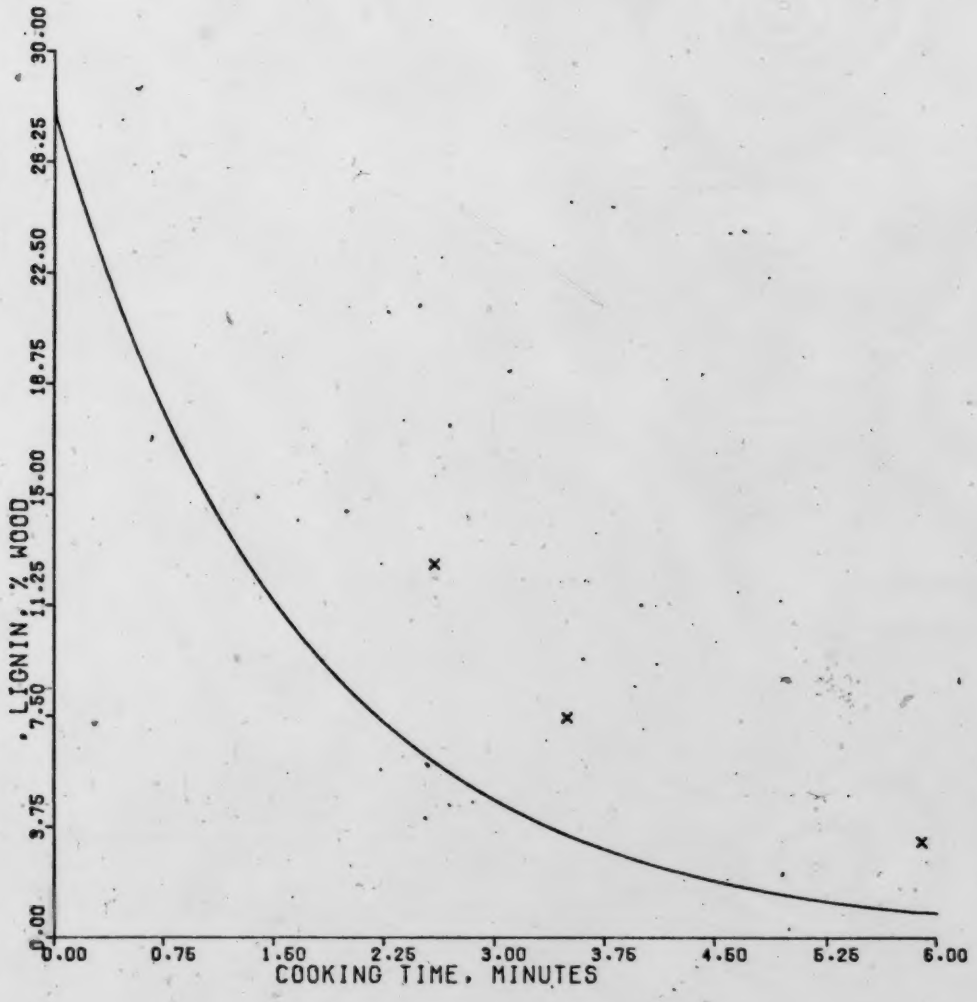


Figure B.2 : Batch Cook, Lignin at 195 °C (Daleski (19))

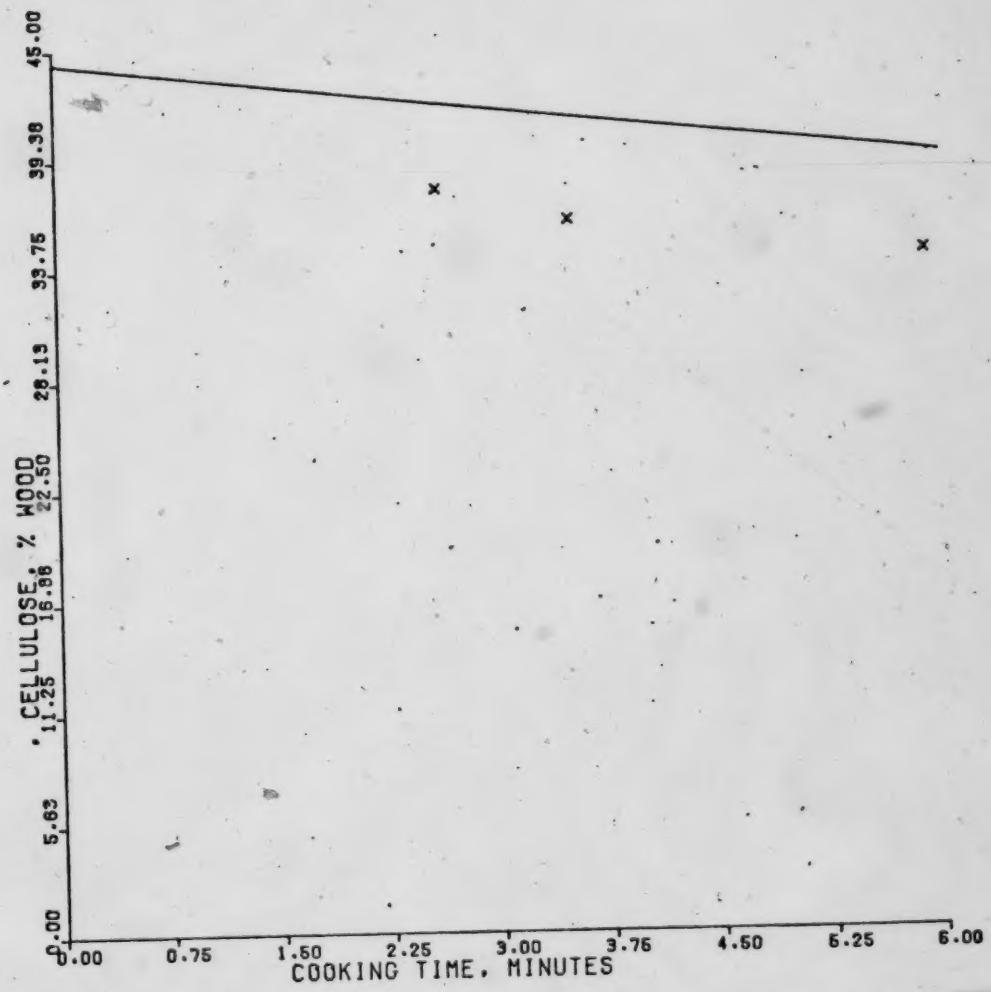


Figure B.3 : Batch Cook, Cellulose at 195 ^{o}C (Daleski (19))

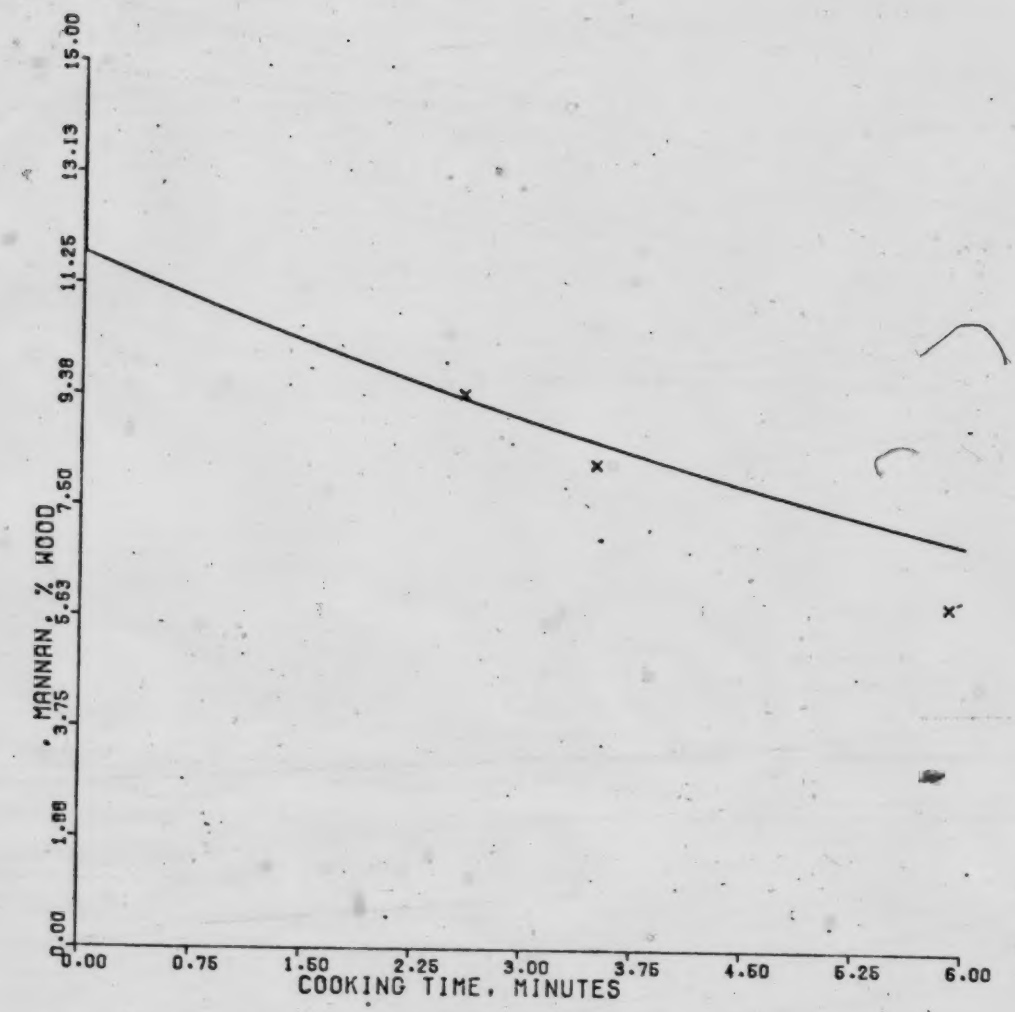


Figure B.4 : Batch Cook, Mannan at 195 °C (Daleski (19))

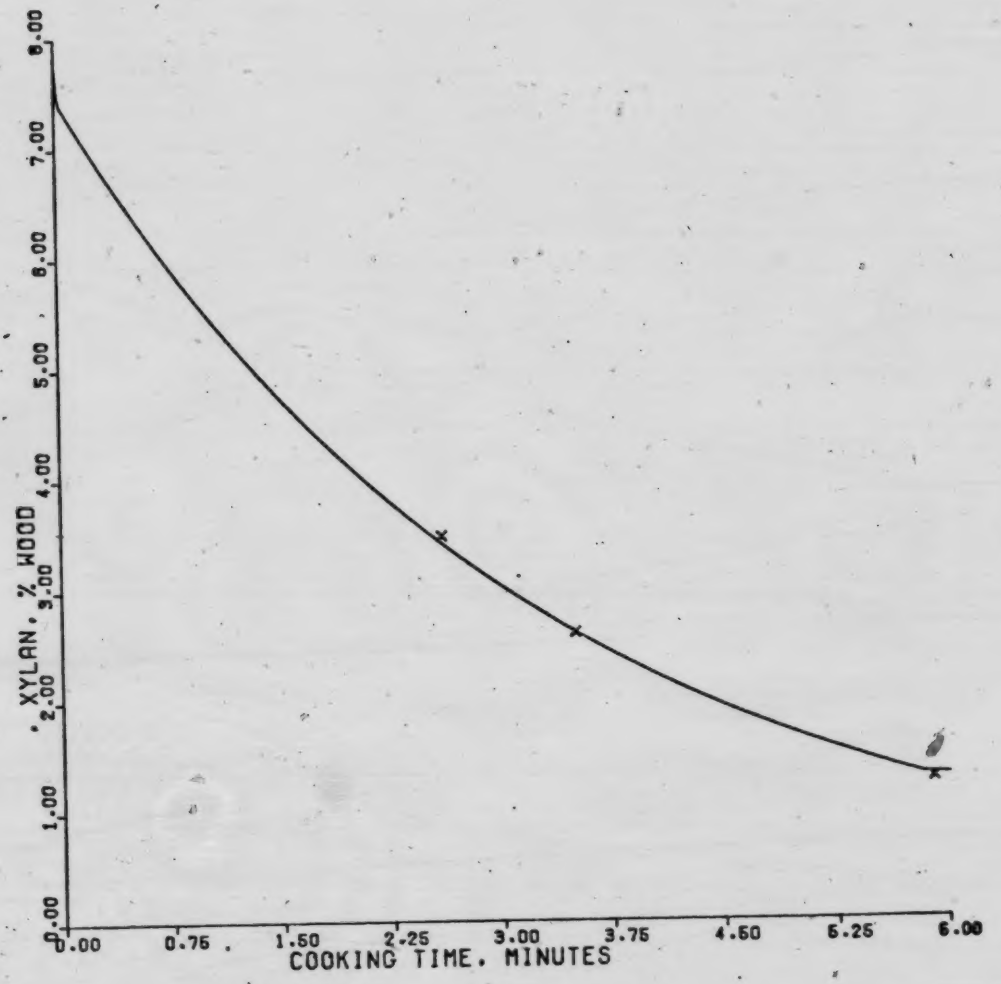


Figure B.5 : Batch Cook, Xylan at 195 ^{o}C (Daleski (19))

APPENDIX C

WORKING OF OPEN LOOP PROGRAM

This appendix contains the flow diagram of the main computer program and a set of sample data with the standard program output. The dynamic and steady state digester models are a part of one program which is about three thousand lines long and the FORTRAN G compiled version on the Amdahl 470/V6 computer occupied a 256K bytes. The run time to generate the profiles in this appendix was 2.5 CPU seconds when the program was already loaded in memory and 3.0 CPU seconds when it was not. The batch program is only 1500 lines long and its compiled version occupied about 100K bytes.

C.1 Open Loop Model Flow Diagram

The flow diagram in this appendix, Figure C.1 is an expanded version of the simplified flow diagram that was shown in Figure 4.1. The more detailed flow diagram with complete program documentation is given in the programmers manual.

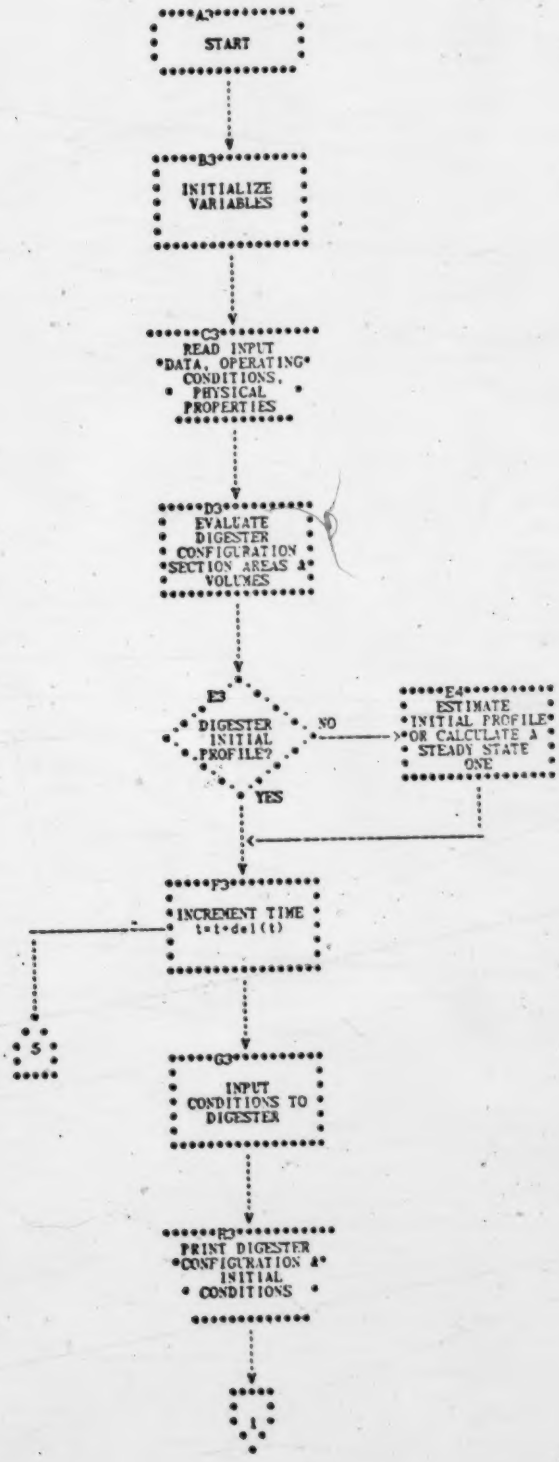


Figure C.1 : Open Loop Model Flow Diagram

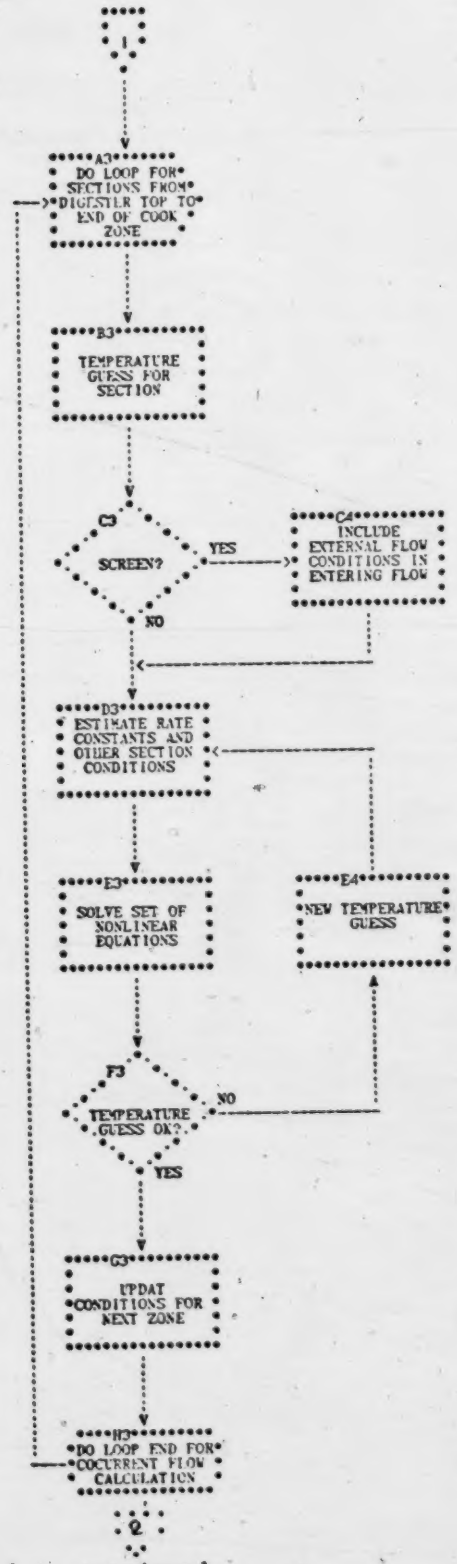


Figure C.1 .. continued

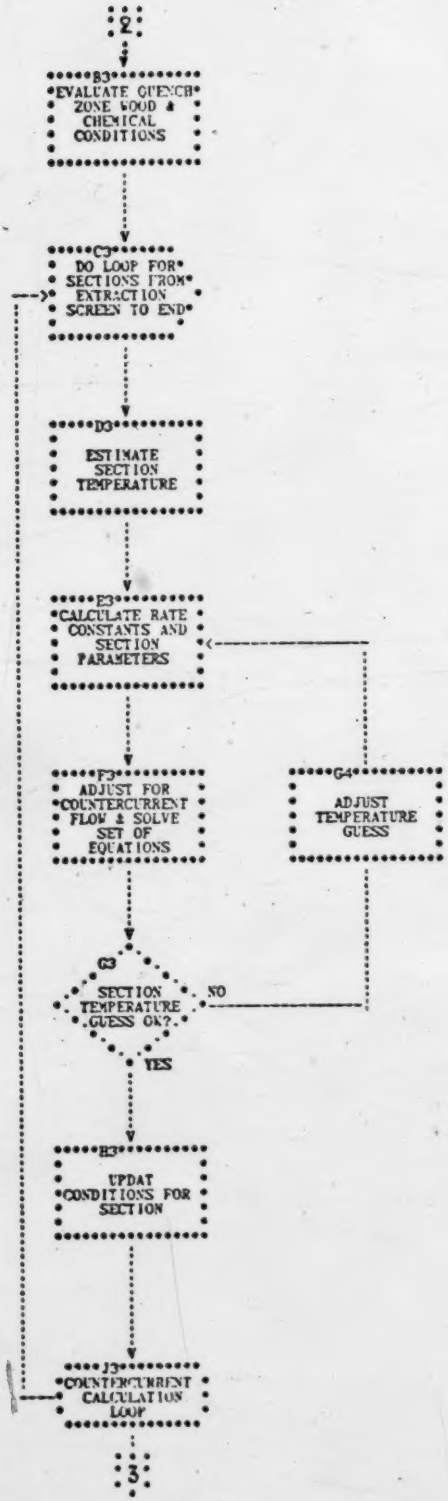


Table C.1 ... continued

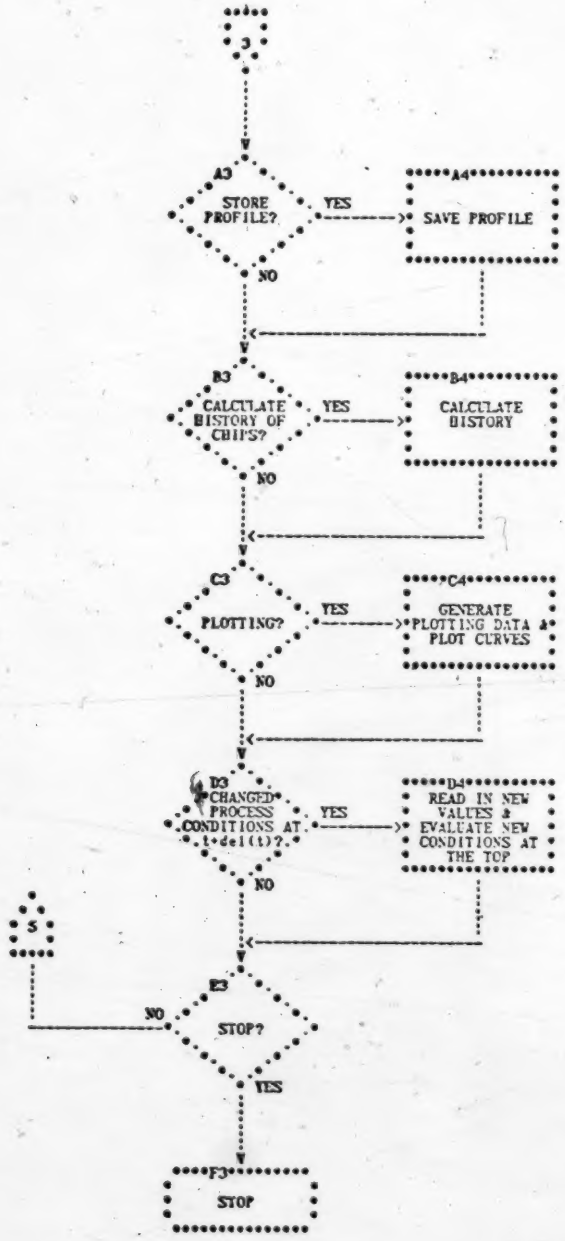


Figure C.1 .. continued

C.2 Open Loop Sample Data and Printout

The data used to produce the results for the sample computer run in the this section is presented here.

Setup of Program Flags

Wood Type	Hardwood
Wood Species	Beech
Units	System Internationale (S.I.)
Initial Profile Type	Startup from scratch
History Required ?	No
Heat Balance ?	No
Secondary Cook?	No
Equation Testing?	No
Changes in Operating Conditions	No
Soda Cook?	No
Rate Constants Readin	Yes
Reaction?	Yes
Washing Calculations?	Yes
Profile Printing Frequency	All
Profile Save Frequency	Every Fourth
Plotting?	Yes
Debugging Messages?	No
Stopping Criterion?	After TOTERO Profiles

** DATA **

Blow Flow	54.0 cu m/min
Pulp Consistency	12.5 %
Chip Flow	63500.0 kg/hr
Chipmeter Capacity	46 kg/revolution
Chip Moisture	50.0 %
Chip Critical Moisture	60.0 %
Wood Specific Area	155.0 sq m/cu m

Dry Wood Density	184.2 kg/cu m
Wood Substance Density	1653.0 kg/cu m
Lignin Content	26.6 kg/100kg ODW
Cellulose Content	39.0 kg/100kg ODW
Mannan Content	16.2 kg/100kg ODW
Xylan Content	9.5 kg/100kg ODW
Acetyls	0.95 kg/100kg ODW
Uronic Acid	3.85 kg/100kg ODW
Extractives	3.90 kg/100kg ODW
Percent Extractive Lignin	15.0 %
Percent Extractive Mannan	55.0 %
Percent Extractive Xylan	15.0 %
White Liquor Flow	12.75 cu m/min
White Liquor Alkali	140.5 kg/cu m as Na2O
White Liquor Sulphidity	33.0 %
White Liquor Solids	0.0 %
White Liquor Temperature	87.0 C
Black Liquor Flow	0.0 cu m/min
Black Liquor Alkali	8.0 kg/cu m
Black Liquor Sulphidity	15.0 %
Black Liquor Solids	3.9 %
Black Liquor Temperature	85.0 C
Upper Heater Flow	30.5 cu m/min
Lower Heater Flow	28.0 cu m/min
Quench Flow	Calculated Latter in Program
Wash Heater Flow	9.0 cu m/min
Upper Heater Temperature	150.0 C
Lower Heater Temperature	155.0 C
Quench Temperature	98.0 C
Wash Heater Temperature	94.0 C
Extraction Flow	35.0 cu m/min
Quench Flow/Extraction Flow Ratio	0.40
Cold Blow Alkali	0.0 kg/cu m
Cold Blow Sulphidity	0.0 %
Cold Blow Solids	0.0 %
Cold Blow Temperature	45.0 C
Kinetic Parameters	Same as in Table 2.

Heat Transfer Coefficients

Internal Pipe and Liquor	0.235 W/sq m - K
Digester Walls	0.0002 W/sq m - K
Free Liquor and Wood	4.72 W/sq m - K

Heat of Reaction	580.0 J/kg of wood reacted
Specific Heat of Wood	2.878 J/kg - K
Specific Heat of Liquor	5.188 J/kg - K
Specific Heat of Ice	2.090 J/kg - K
Heat of Fusion of Ice	93.0 J/kg
Heat of Condensation of Steam	2188.0 J/kg
Temperature of Chips	30.0 C
Temperature of Steaming Vessel	125.0 C
Ambient Temperature	29.0 C
Digester Dimensions	Printed out in Sample Outpu

Number of Sections per Zone

Impregnation	3
Upper Heater	2
Lower Heater	Always 1
Cooking	6
Quench	Always 1
Extraction	Always 1
Washing	7+1 for Wash heater screen
Cold Blow	2

Numerical Step Size	5.0 min
Profiles to be Calculated	2

Limit Checking constants for Variables

Every Profile Plotted?	No
Number of Variables Plotted	6
Total Number of Plots	1
Profile Number of Plot	1

Variables to be Plotted

Lignin
Cellulose
Mannan
Xylan
Entrapped Hydroxide
Chip Temperature

C.3 Documentation Produced by the Computer Program

The sample computer run follows and consists of the digester configuration, volumes and areas in each section, initial digester entering flows, the initial digester profile and the dynamic profiles. The plots and other output from a similar run were shown in chapter five. Details are given in the programmer's manual.

Table C.1 : Open Loop Sample Data and Run

```
      1     1,1,-2,0,0,0;
      2     0,0,0,1,1,1;
      3     1,10,1,0,0,0;
      4     54.0,12.5,63500.0,46.0,50.0,60.0,213.25;
      5     HARDWOOD   BEECH
      6     184.5,1653.0,1653.0,1653.0,1653.0;
      7     26.6,39.0,16.2,9.5,0.95,3.85,3.90,15.0,55.0,15.0;
      8     9.95,0.0,128.4,8.5,33.0,15.0,0.0,9.9,87.0,85.0;
      9     30.5,150.0,28.0,155.0,0.0,98.0,9.0,94.0,0.4,14.8;
     10     0.0,0.0,0.0,45.0;
     11     0.235,0.002,4.72,580.0,580.0,580.0,580.0,0.0;
     12     2.88,5.24,2.05,93.0,30.0,125.0,2188.0,29.0;
     13     4.10,4.85,4.85,4.95,5.00,5.10,4.85,4.80,4.75;
     14     37.5,55.75,50.0,50.0,45.0,40.0,40.0,40.0;
     15     4.80,10.0,3.25,1.90,18.50,2.35,2.60,23.0,3.90,1.30,2.50;
     16     3,2,1,6,1,1,8,2;
     17     1.65,1.35,1.15;
     18     1.0,1.0,0.1,0.01,0.09,0.1,0.07,1.4,100.0;
     19     1,1;
     20     0.0,20.0,2.0,320.0,85.0,0.05,2.0,0.0,0.0,0.0,0.0,85.0,450.0,1200.0,0.0;
     21     400.0,100.0,0.5,80000.0,2.0,2.0,20.0,250.0,65.0,50.0,250.0,2000.0;
     22     0,6;
     23     14;
     24     1,20,50,100,150,200,250,300,350,400,450,500,550,600;
     25     2,3,4,5,6,9;
     26     2;
     27     1,2;
     28     21;
END OF FILE
```

Table C.1 ... continued

**** CONFIGURATION OF THE DIGESTER ****

TOTAL HEIGHT OF DIGESTER, M
70.30
TOTAL VOLUME CU. M
1265.86

ZONE HEIGHTS, M

IMPREGNATION	14.80
UPPER HEATING	3.25
LOWER HEATING	1.90
COOKING	18.50
QUENCH	2.35
EXTRACTION	2.60
WASHING	23.00
COLD BLOW	3.90

INSIDE DIAMETER AND HEIGHT OF DIGESTER ZONES, M

TOP OF CONE	BOTTOM OF CONE	D(3)	D(4)	D(5)	D(6)	D(7)	D(8)	D(9)
4.10	4.85	4.85	4.95	5.00	5.10	4.85	4.80	4.75
4.80	10.00	3.25	1.90	18.50	2.35	2.60	23.00	3.90

OUTSIDE DIAMETERS OF PIPE BUNDLE, CM

DP(1)	DP(2)	DP(3)	DP(4)	DP(5)	DP(6)	DP(7)	DP(8)
37.50	55.75	50.00	50.00	45.00	40.00	40.00	40.00

*** SECTION CONFIGURATION ***

ZONE	SECTION AND SCREEN NO.	VOLUME CU. M	PIPE AREA SQ. M	WALL AREA SQ. M
IMPG	1	32.61	2.64	29.56
	2	25.03	4.10	20.91
	3	181.68	29.29	152.37
UPHT	4	29.98	4.53	25.14
	SCREEN 1			
	5	29.07	4.40	24.38
LHET	6	31.25	4.53	25.66
	SCREEN 2			
CKNG	7	59.71	7.99	48.43
	8	59.71	7.99	48.43
	9	59.71	7.99	48.43
	10	59.71	7.99	48.43
	11	59.71	7.99	48.43
	12	59.71	7.99	48.43
QUEN	13	47.71	2.95	37.65
	SCREEN 3			
EXTR	14	47.71	3.27	39.62
	SCREEN 4			
WASH				
	15	56.09	3.92	47.07
	16	56.09	3.92	47.07
	17	56.09	3.92	47.07
	18	56.09	3.92	47.07
	19	56.09	3.92	47.07
	20	56.09	3.92	47.07
	21	56.09	3.92	47.07
	22	20.81	0.0	17.34
	SCREEN 5			
CBLO	23	34.56	0.0	29.10
	24	34.56	0.0	29.10

Table C.1 ... continued

**** INITIAL CONCENTRATIONS AND FLOWS ****
ENTERING THE DIGESTER

****
* WOOD/ PULP *
****

SPECIE	TYPE	CHIP FLOW KGS ODW/HR	MOISTURE WT PERCENT	BLOW FLOW CU M/MIN	CONSISTENCY WT PERCENT
HARDWOOD	BEECH	63500.0	50.00	54.00	12.50

LIGNIN	CELLULOSE	MANNAN	XYLAN	OTHERS
KGS / 100 KGS OF OVEN DRY WOOD				
26.600	39.000	16.200	9.500	8.700

****
* COOKING CHEMICALS *
****

BLACK LIQUOR		WHITE LIQUOR	
FLOW CU M/MIN	TEMP DEGREE C	FLOW CU M/MIN	TEMP DEGREE C
0.0	85.00	9.95	87.00

ENTERING DIGESTER FREE LIQUOR

FLOW	NAOH	NA2S	SOLIDS	COND FLOW	TEMP
CU M/MIN	KG/CU M	KG/CU M	KG/CU M	CU M/MIN	DEGREE C
9.53	87.21	42.95	0.0	1.49	91.92

Table C.1 ... continued

DIGESTER CONDITIONS AT TIME ZERO

WOOD RATE KG ODW/MIN	LIGNIN KG OF WOOD	CELLULOSE COMPONENT/100 KG	MANNAN OD WOOD	XYLAN	ELHYD ------	ELSUL CONCENTRATION	ELPRO OF LIQUOR	FLHYD COMPONENT	FLSUL KG/CU M------	FLPRO	TEMP DEGREE C
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	91.92
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	91.92
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	91.92
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	141.61
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	141.61
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	146.36
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	92.21
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	97.42
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	88.41
2745.695	26.600	39.000	16.200	9.500	12.862	6.335	0.0	87.207	42.953	0.0	45.31

Table Table C.1 ... continued

DIGESTER PROFILE AT 1.000 MINS

| HARDWOOD TYPE IN USE : SPECIE BEECH |

KG OF WOOD COMPONENT /100 KG OD WOOD				CONCENTRATION OF LIQUOR COMPONENT KG/CU M						DEGREES C	
LIGNIN	CELLULOSE	MANNAN	XYLAN	NAOH		NA2S		REACTION PRODUCT		TEMP	K-NO
26.590	39.000	16.165	9.498	12.999	86.625	6.443	42.905	3.877	0.003	91.92	44.19
26.590	39.000	16.166	9.498	13.000	86.533	6.443	42.909	4.933	0.003	91.92	44.19
26.589	39.000	16.164	9.498	13.024	86.989	6.456	42.897	1.126	0.001	91.92	44.19
26.517	39.000	15.939	9.487	12.740	87.015	6.585	42.858	3.095	0.005	141.61	44.15
25.342	38.993	12.933	9.324	5.326	86.471	6.571	42.613	40.246	0.229	141.61	43.54
25.143	38.992	12.513	9.298	4.237	86.417	6.533	42.591	45.693	0.279	146.36	43.43
24.760	38.989	11.727	9.248	2.208	86.184	6.464	42.490	56.057	0.423	146.36	43.22
24.753	38.990	11.762	9.250	2.299	86.133	6.463	42.467	55.766	0.442	146.36	43.22
24.746	38.990	11.795	9.253	2.382	86.079	6.463	42.442	55.501	0.463	146.36	43.22
24.740	38.990	11.825	9.255	2.459	86.022	6.463	42.416	55.256	0.484	146.36	43.21
24.734	38.990	11.853	9.257	2.530	85.963	6.463	42.389	55.030	0.507	146.36	43.21
24.729	38.990	11.879	9.259	2.596	85.900	6.463	42.360	54.819	0.531	146.36	43.21
26.290	38.998	15.341	9.500	11.442	86.526	6.664	42.623	10.452	0.054	92.21	44.03
26.586	39.000	16.160	9.500	13.025	87.095	6.461	42.898	0.485	0.000	97.42	44.18
26.591	39.000	16.173	9.500	13.030	87.106	6.448	42.903	0.327	0.000	88.41	44.19
26.591	39.000	16.173	9.500	13.031	87.106	6.448	42.903	0.325	0.000	88.41	44.19
26.591	39.000	16.173	9.500	13.031	87.106	6.448	42.903	0.324	0.000	88.41	44.19
26.591	39.000	16.174	9.500	13.031	87.106	6.448	42.903	0.322	0.000	88.41	44.19
26.591	39.000	16.174	9.500	13.032	87.106	6.448	42.903	0.321	0.000	88.41	44.19
26.591	39.000	16.174	9.500	13.032	87.106	6.448	42.903	0.319	0.000	88.41	44.19
26.591	39.000	16.174	9.500	13.033	87.106	6.448	42.903	0.318	0.000	88.41	44.19
26.591	39.000	16.176	9.500	13.016	87.126	6.438	42.913	0.287	0.000	88.41	44.19
26.591	39.000	16.175	9.500	13.027	87.114	6.444	42.907	0.305	0.000	88.41	44.19
26.599	39.000	16.197	9.500	12.961	55.778	6.387	27.473	0.040	0.000	45.31	44.19